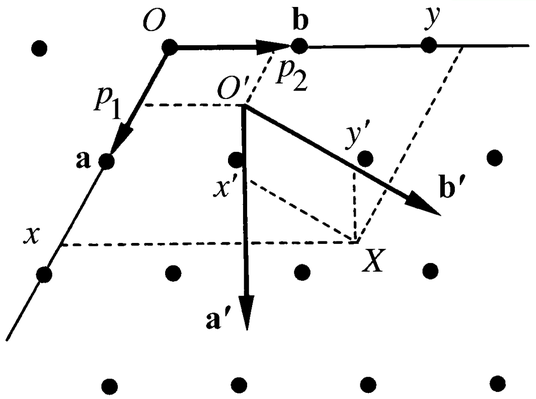
University of Science and Technology, Beijung
Optical Material and Device Lab

2022 SPRING FESTIVAL BEIJING CRYSTALLOGRAPHY SCHOOL

February 1 - 14, Beijing 2022

CO-ORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY

Co-ordinate transformation



3-dimensional space

$(\mathbf{a}, \mathbf{b}, \mathbf{c})$, origin O: point $\mathrm{X}(x, y, z)$

(P,p) ↓

$(\mathbf{a}', \mathbf{b}', \mathbf{c}')$, origin O': point $\mathrm{X}(x', y', z')$

Transformation matrix-column pair (P,p)

(i) linear part: change of orientation or length:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$$

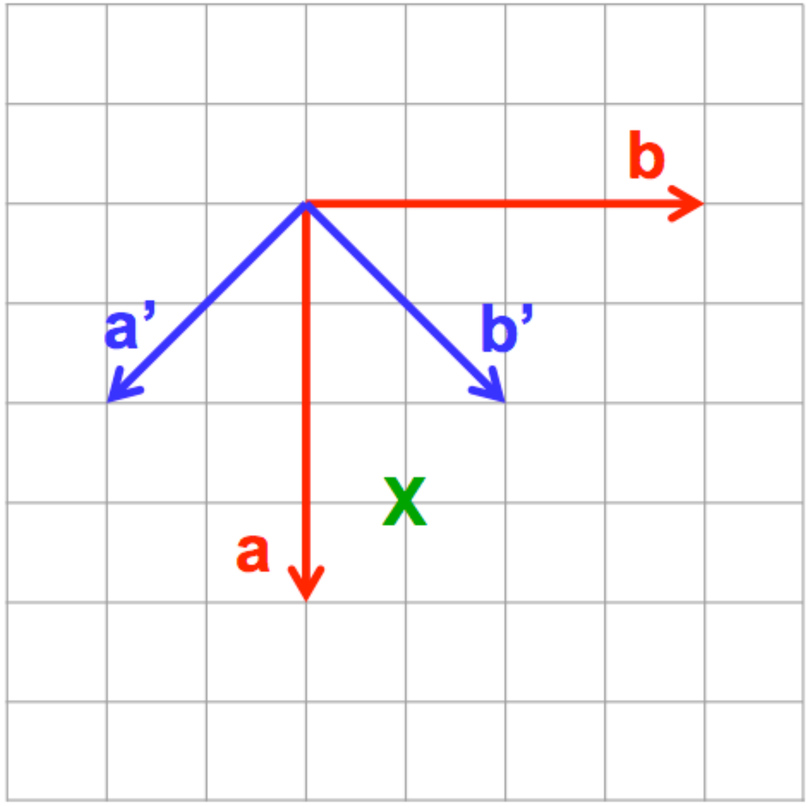
$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c},$$
$$P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c},$$
$$P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}).$$

(ii) origin shift by a shift vector $\boldsymbol{p}(p_1,p_2,p_3)$:

$$\boldsymbol{O' = O + p}$$

the origin ***O'*** has coordinates (p_1,p_2,p_3) in the old coordinate system

EXAMPLE



$$(a',b',c') = (a,b,c)\begin{pmatrix} ? \end{pmatrix}$$

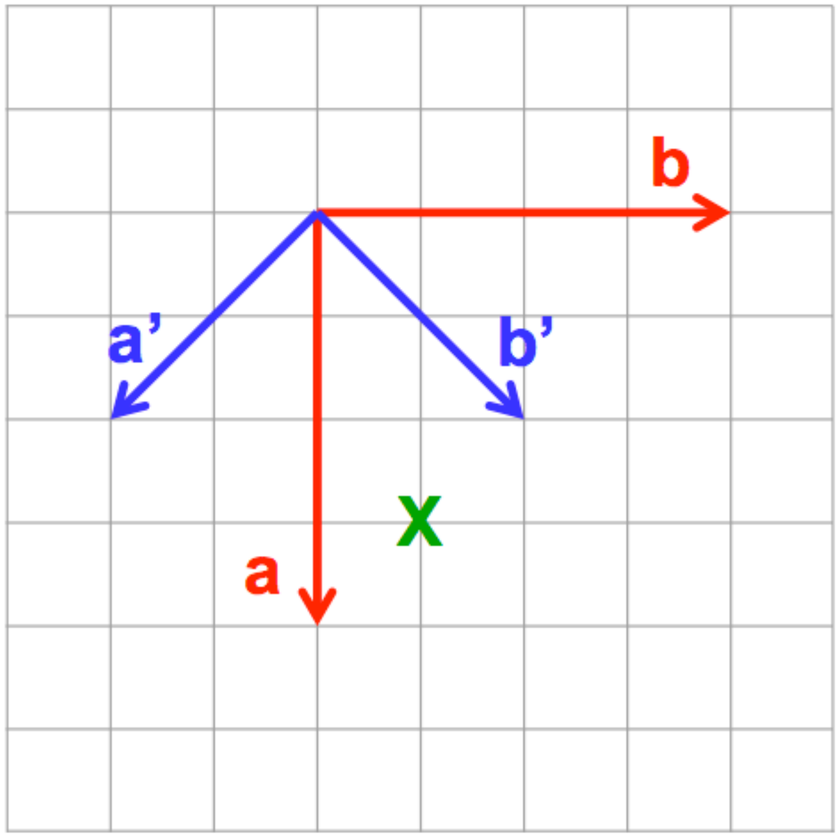
$$(a,b,c) = (a',b',c')\begin{pmatrix} ? \end{pmatrix}$$

$$X = (3/4, 1/4, 0)$$

$$X' = (\ ?\ )$$

Write "new in terms of old" as column vectors.

QUICK QUIZ



SOLUTION

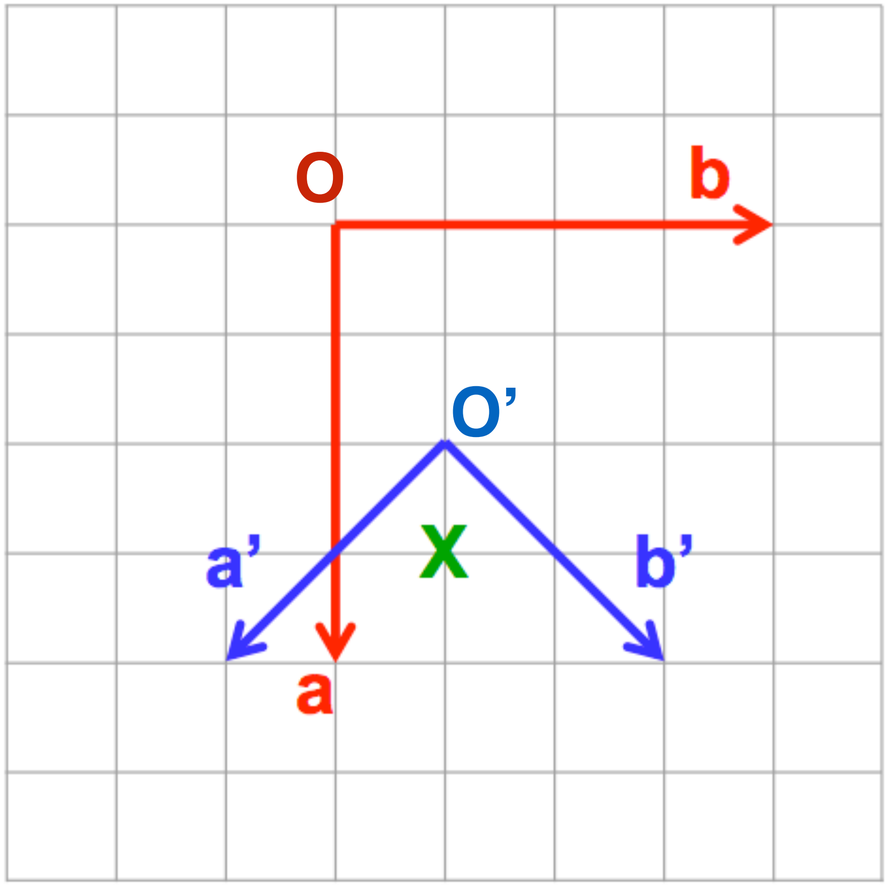
$$(a',b',c') = (a,b,c)\begin{pmatrix} 1/2 & 1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(a,b,c) = (a',b',c')\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$X = (3/4,1/4,0)$$

$$X' = (1/2,1,0)$$

EXAMPLE



$$p = \begin{pmatrix} ? \end{pmatrix}$$

$$q = \begin{pmatrix} ? \end{pmatrix}$$

$$X = (3/4, 1/4, 0)$$

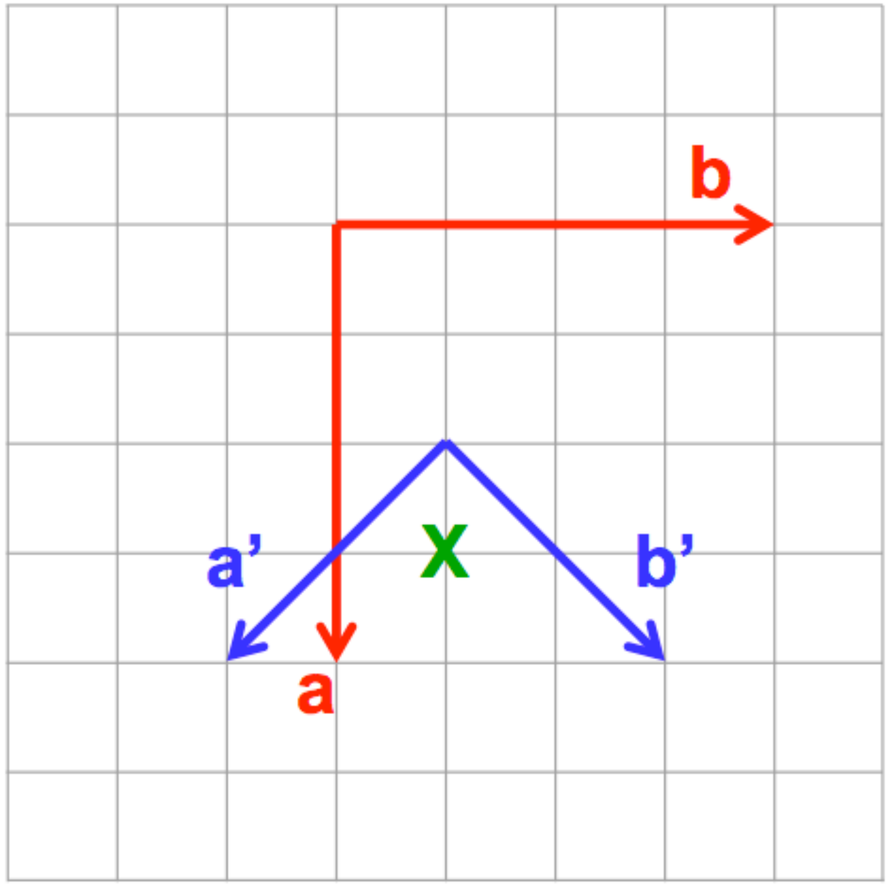
$$X' = (\ ?\ )$$

O’= O + p

Linear parts as before.

QUICK QUIZ

SOLUTION



$$\boldsymbol{p} = \begin{pmatrix} 1/2 \\ 1/4 \\ 0 \end{pmatrix}$$

$$\boldsymbol{q} = \begin{pmatrix} -1/4 \\ -3/4 \\ 0 \end{pmatrix}$$

$$\boldsymbol{X} = (3/4, 1/4, 0)$$

$$\boldsymbol{X}' = (1/4, 1/4, 0)$$

Linear parts as before.

Transformation matrix-column pair (*P,p*)

$$(P,p)=\left(\begin{array}{ccc|c} 1/2 & 1/2 & 0 & 1/2 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{array}\right)$$

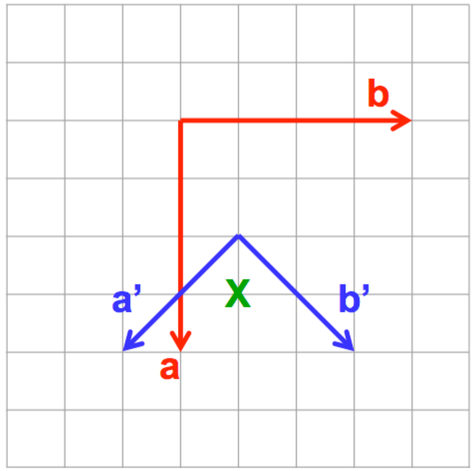
$$(P,p)^{-1}=\left(\begin{array}{ccc|c} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -3/4 \\ 0 & 0 & 1 & 0 \end{array}\right)$$

a'=1/2a-1/2b

b'=1/2a+1/2b

c'=c

$$O'=O+\begin{pmatrix}1/2\\1/4\\0\end{pmatrix}$$



a=a'+b'

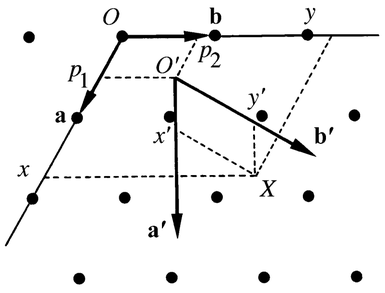
b=-a'+b'

c=c'

$$O=O'+\begin{pmatrix}-1/4\\-3/4\\0\end{pmatrix}$$

Short-hand notation for the description of transformation matrices

Transformation matrix:



(**a**,**b**,**c**), origin O

$$(P,p)=\left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p1 \\ P_{21} & P_{22} & P_{23} & p2 \\ P_{31} & P_{32} & P_{33} & p3 \end{array}\right)$$

(**a'**,**b'**,**c'**), origin O'

notation rules:

-written by columns
-coefficients 0, +1, -1
-different columns in one line
-origin shift

example:

1	-1		-1/4
1	1		-3/4
		1	0

⟶ { a+b, -a+b, c;-1/4,-3/4,0

Transformation of the coordinates of a point X(x,y,z):

$$(X')=(P,p)^{-1}(X)$$
$$=(P^{-1}, -P^{-1}p)(X)$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p1 \\ P_{21} & P_{22} & P_{23} & p2 \\ P_{31} & P_{32} & P_{33} & p3 \end{array} \right)^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

special cases

-origin shift (***P***=***I***):

$$x' = x - p$$

-change of basis (***p***=***o***) :

$$x' = P^{-1}x$$

EXAMPLE

$$X'=(P,p)^{-1}X= \left(\begin{array}{ccc|c} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -3/4 \\ 0 & 0 & 1 & 0 \end{array} \right) \begin{pmatrix} 3/4 \\ 1/4 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix}$$

QUICK QUIZ

Determine the coordinates X' of a point X= with respect to the new basis
(**a'**,**b'**,**c'**)= (**a**,**b**,**c**)**P**, with **P**=**c**,**a**,**b**.

0,70
0,31
0,95

Hint

$$(X')=(P,p)^{-1}(X)$$

Covariant and contravariant crystallographic quantities

direct or crystal basis

$$(\mathbf{a'},\mathbf{b'},\mathbf{c'})=(\mathbf{a},\mathbf{b},\mathbf{c})P=(\mathbf{a},\mathbf{b},\mathbf{c})\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

reciprocal or dual basis

$$\begin{pmatrix} \mathbf{a^{*'}} \\ \mathbf{b^{*'}} \\ \mathbf{c^{*'}} \end{pmatrix} = P^{-1}\begin{pmatrix} \mathbf{a^{*}} \\ \mathbf{b^{*}} \\ \mathbf{c^{*}} \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}^{-1}\begin{pmatrix} \mathbf{a^{*}} \\ \mathbf{b^{*}} \\ \mathbf{c^{*}} \end{pmatrix}$$

covariant to crystal basis: Miller indices

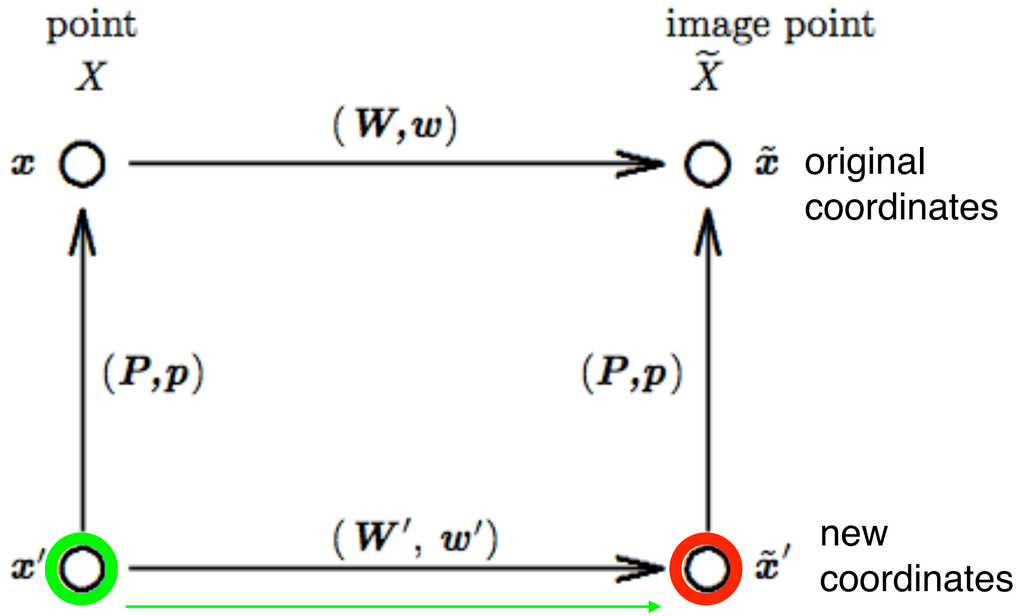
$$(h',k',l')=(h,k,l)P$$

contravariant to crystal basis: indices of a direction [u]

$$\begin{pmatrix} \mathbf{u'} \\ \mathbf{v'} \\ \mathbf{w'} \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}^{-1}\begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

Transformation of symmetry operations (W,w)

$$(W',w')=(P,p)^{-1}(W,w)(P,p)$$



i. $\tilde{x}' = (W', w')x'$.

ii. $\tilde{x}' = (P,p)^{-1}\tilde{x} = (P,p)^{-1}(W,w)x = (P,p)^{-1}(W,w)(P,p)x'$.

Transformation of the coordinates of a point X(x,y,z):

$$(X')=(P,p)^{-1}(X)$$
$$=(P^{-1}, -P^{-1}p)(X)$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p1 \\ P_{21} & P_{22} & P_{23} & p2 \\ P_{31} & P_{32} & P_{33} & p3 \end{array} \right)^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

special cases

-origin shift (***P***=***I***):

$$x' = x - p$$

-change of basis (***p***=***o***) :

$$x' = P^{-1}x$$

Transformation of symmetry operations (*W,w*):

$$(W',w')=(P,p)^{-1}(W,w)(P,p)$$

Transformation by (***P***,***p***) of the unit cell parameters:

metric tensor ***G***: $G' = P^t G P$

Problem: SYMMETRY DATA
ITA SETTINGS

530 ITA settings of **orthorhombic** and **monoclinic** groups

Table 4.3.1 (*cont.*)

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						Unique axis *b* Unique axis *c* Unique axis *a*
			a<u>b</u>c	**c<u>b̄</u>a**	**ab<u>c</u>**	**ba<u>c̄</u>**	**<u>a</u>bc**	**<u>ā</u>cb**	
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121$ $A121$ $I121$	$A121$ $C121$ $I121$	$A112$ $B112$ $I112$	$B112$ $A112$ $I112$	$B211$ $C211$ $I211$	$C211$ $B211$ $I211$	Cell choice 1 Cell choice 2 Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$ $P1n1$ $P1a1$	$P1a1$ $P1n1$ $P1c1$	$P11a$ $P11n$ $P11b$	$P11b$ $P11n$ $P11a$	$Pb11$ $Pn11$ $Pc11$	$Pc11$ $Pn11$ $Pb11$	Cell choice 1 Cell choice 2 Cell choice 3
8	C_s^3	Cm	$C1m1$ $A1m1$ $I1m1$	$A1m1$ $C1m1$ $I1m1$	$A11m$ $B11m$ $I11m$	$B11m$ $A11m$ $I11m$	$Bm11$ $Cm11$ $Im11$	$Cm11$ $Bm11$ $Im11$	Cell choice 1 Cell choice 2 Cell choice 3
9	C_s^4	Cc	$C1c1$ $A1n1$ $I1a1$	$A1a1$ $C1n1$ $I1c1$	$A11a$ $B11n$ $I11b$	$B11b$ $A11n$ $I11a$	$Bb11$ $Cn11$ $Ic11$	$Cc11$ $Bn11$ $Ib11$	Cell choice 1 Cell choice 2 Cell choice 3
10	C_{2h}^1	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	C_{2h}^2	$P2_1/m$	$P1\frac{2_1}{m}1$	$P1\frac{2_1}{m}1$	$P11\frac{2_1}{m}$	$P11\frac{2_1}{m}$	$P\frac{2_1}{m}11$	$P\frac{2_1}{m}11$	

SYMMETRY DATA: ITA SETTINGS

Monoclinic descriptions

	Transf.	**abc**	**cb̄a**	**abc**	**ba$\bar{c}$**	**abc**	**ā$\bar{c}$b**	Monoclinic axis b Monoclinic axis c Monoclinic axis a
HM	$C2/c$	$C12/c1$ $A12/n1$ $I12/a1$	$A12/a1$ $C12/n1$ $I12/c1$	$A112/a$ $B112/n$ $I112/b$	$B112/b$ $A112/n$ $I112/a$	$B2/b11$ $C2/n11$ $I2/c11$	$C2/c11$ $B2/n11$ $I2/b11$	Cell type 1 Cell type 2 Cell type 3

Orthorhombic descriptions

No.	HM	**abc**	**ba$\bar{c}$**	**cab**	**c̄ba**	**bca**	**ac̄b**
33	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$

FCT/ZTF

bilbao crystallographic server

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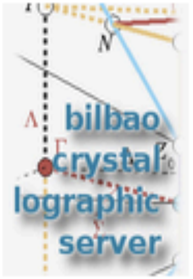

ECM31-Oviedo Satellite

Crystallography online: workshop on
use and applications of the structural t
of the Bilbao Crystallographic Serve

20-21 August 2018

News:

- **New Article in Nature**
  07/2017: Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017). **547**, 298-305.
- **New program: BANDREP**
  04/2017: Band representations and Elementary Band representations of Double Space Groups.
- **New section: Double point and space groups**
  - **New program: DGENPOS**
    04/2017: General positions of Double Space Groups
  - **New program: REPRESENTATIONS DPG**

Space-group symmetry

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

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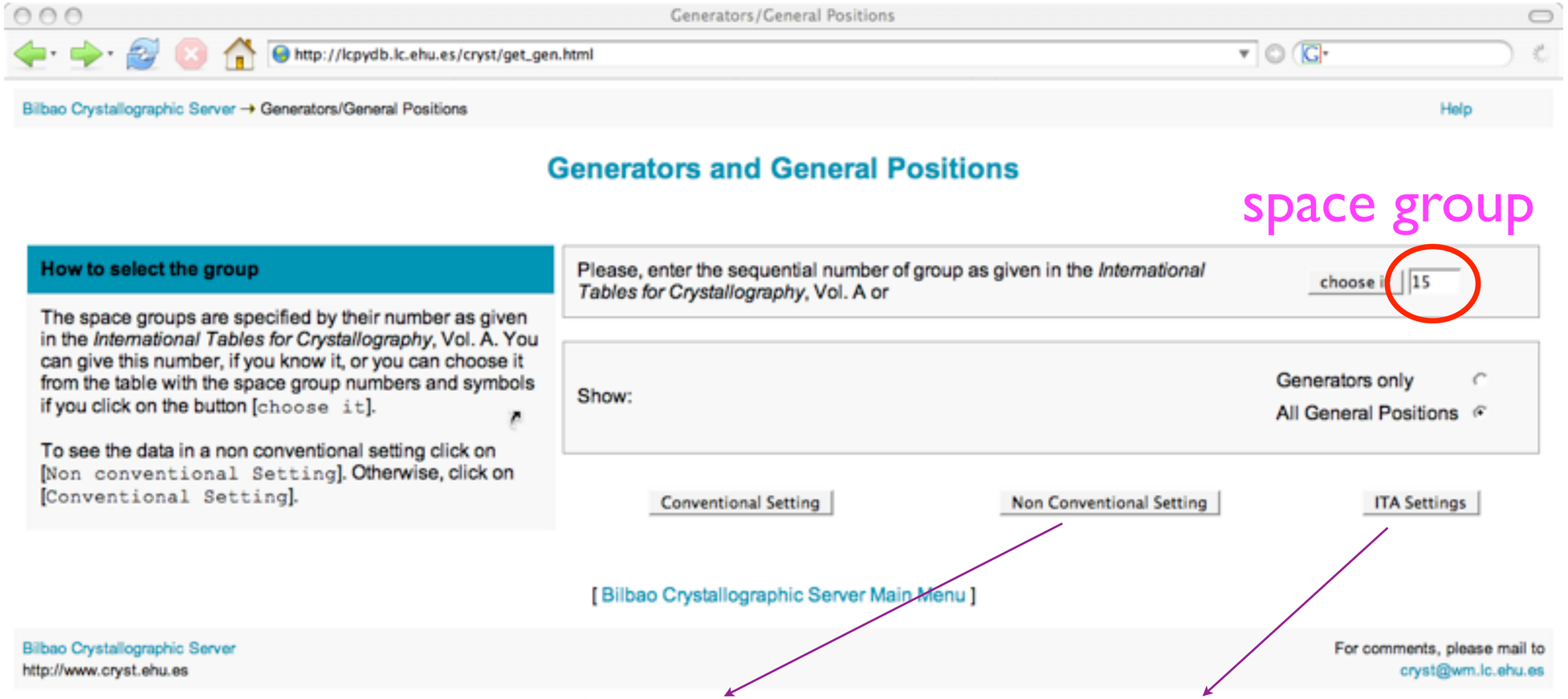
Problem: Coordinate transformations
Generators
General positions

GENPOS



Transformation of the basis

ITA-settings symmetry data

ITA-Settings for the Space Group 15

Note: The transformation matrices must be read by columns. **P** is the transformation from standard to the ITA-setting.

$$(a, b, c)_n = (a, b, c)_s \, P$$

ITA number	Setting	P	P^{-1}
15	*C* 1 2/*c* 1	a,b,c	a,b,c
15	*A* 1 2/*n* 1	-a-c,b,a	c,b,-a-c
15	*I* 1 2/*a* 1	c,b,-a-c	-a-c,b,a
15	*A* 1 2/*a* 1	c,-b,a	c,-b,a
15	*C* 1 2/*n* 1	a,-b,-a-c	a,-b,a-c
15	*I* 1 2/*c* 1	-a-c,-b,c	-a-c,-b,c
15	*A* 1 1 2/*a*	c,a,b	b,c,a
15	*B* 1 1 2/*n*	a,-a-c,b	a,c,-a-b
15	*I* 1 1 2/*b*	-a-c,c,b	-a-b,c,b
15	*B* 1 1 2/*b*	a,c,-b	a,-c,b
15	*A* 1 1 2/*n*	-a-c,a,-b	b,-c,-a-b
15	*I* 1 1 2/*a*	c,-a-c,-b	-a-b,-c,a
15	*B* 2/*b* 1 1	b,c,a	c,a,b
15	*C* 2/*n* 1 1	b,a,-a-c	b,a,-b-c
15	*I* 2/*c* 1 1	b,-a-c,c	-b-c,a,c
15	*C* 2/*c* 1 1	-b,a,c	b,-a,c
15	*B* 2/*n* 1 1	-b,-a-c,a	c,-a,-b-c
15	*I* 2/*b* 1 1	-b,c,-a-c	-b-c,-a,b

Example GENPOS:

default setting C12/c1

$(W,w)_{A112/a} = (P,p)^{-1}(W,w)_{C12/c1}(P,p)$

final setting A112/a

Example GENPOS: ITA settings of C2/c(15)

The general positions of the group 15 (*A* 1 1 2/*a*)

N	Standard/Default Setting *C2/c*			ITA-Setting *A* 1 1 2/*a*		
	(x,y,z) form	matrix form	symmetry operation	(x,y,z) form	matrix form	symmetry operation
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
2	-x, y, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 0,y,1/4	-x+1/2, -y, z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 1/4,0,z
3	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0
4	x, -y, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c x,0,z	x+1/2, y, -z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	a x,y,0
5	x+1/2, y+1/2, z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	t (1/2,1/2,0)	x, y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	t (0,1/2,1/2)
6	-x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 1/4,y,1/4	-x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 1/4,1/4,z
7	-x+1/2, -y+1/2, -z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 1/4,1/4,0	-x, -y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-1 0,1/4,1/4
8	x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	n (1/2,0,1/2) x,1/4,z	x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	n (1/2,1/2,0) x,y,1/4

default setting ***A* 1 1 2/*a* setting**

Bilbao Crystallographic Server

Problem: Coordinate transformations Wyckoff positions WYCKPOS

Wyckoff Positions

space group

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

If you are using this program in the preparation of a paper, please cite it in the following form:

Aroyo, *et. al. Zeitschrift fuer Kristallographie* (2006), **221**, 1, 15-27.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

Transformation of the basis

ITA settings

ITA-Settings for the Space Group 68

ces must be read by columns. **P** is the transformation f

$(a, b, c)_n = (a, b, c)_s P$

ITA number	Setting	P	P^{-1}
68	*C c c* e [origin 1]	a,b,c	a,b,c
68	*A* e *a a* [origin 1]	c,a,b	b,c,a
68	*B b* e *b* [origin 1]	b,c,a	c,a,b
68	*C c c* e [origin 2]	a,b,c	a,b,c
68	*A* e *a a* [origin 2]	c,a,b	b,c,a
68	*B b* e *b* [origin 2]	b,c,a	c,a,b

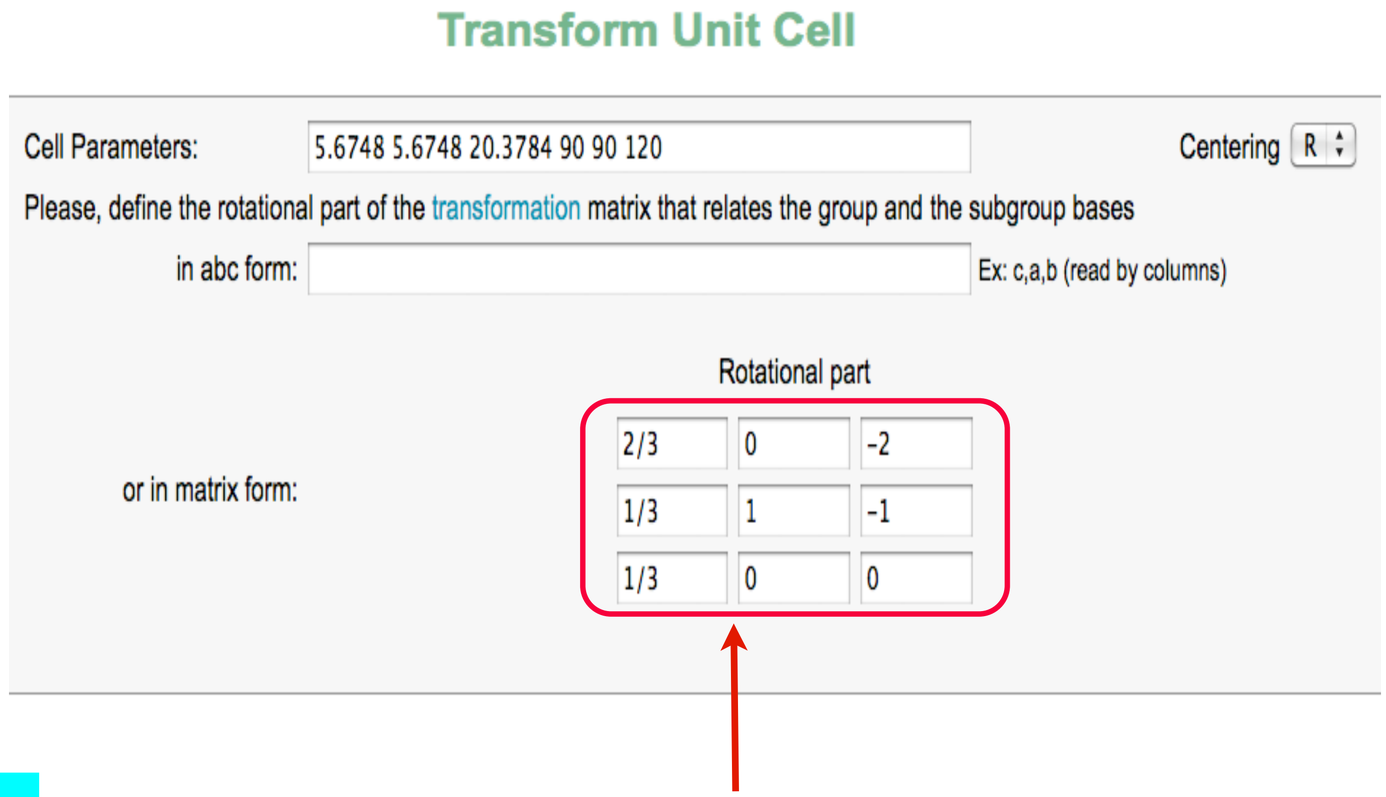
Bilbao Crystallographic Server

Problem: UNIT CELL TRANSFORMATION **CELLTRAN**

lattice parameters hexagonal cell

$G' = P^T G P$

lattice parameters monoclinic cell



(P,p) Transformation matrix

METRIC TENSOR

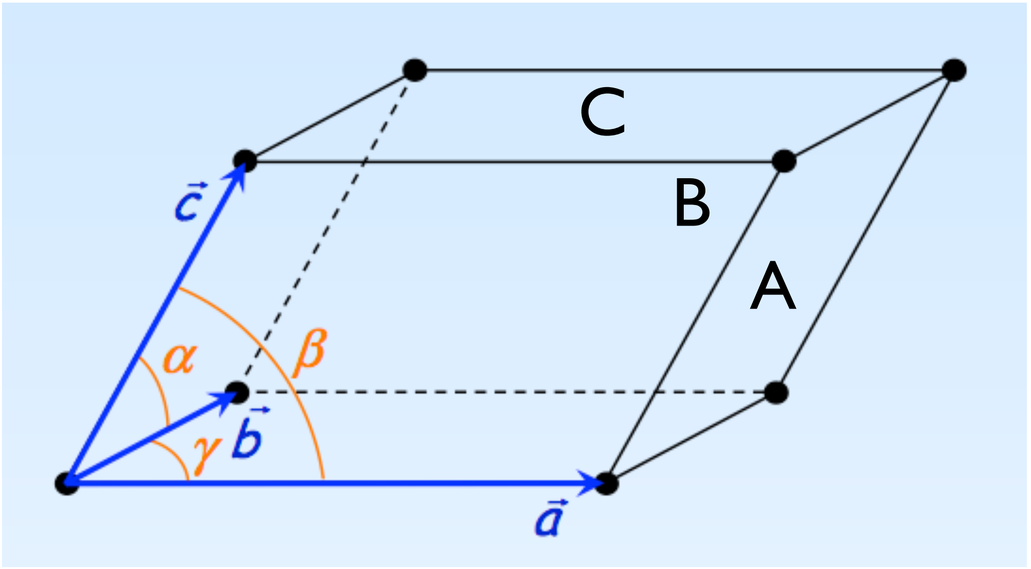
BOND LENGTHS

BONDING ANGLES

3D-unit cell and lattice parameters

lattice basis:
{**a**, **b**, **c**}

***unit cell*:**
the parallelepiped defined by the basis vectors



primitive P and **centred** unit cells:
A,B,C,F, I, R

number of lattice points per unit cell

Lattice parameters

lengths of the unit translations:

a

b

c

angles between them:

$\alpha = (\vec{b}, \vec{c})$

$\beta = (\vec{c}, \vec{a})$

$\gamma = (\vec{a}, \vec{b})$

METRIC TENSOR (FUNDAMENTAL MATRIX)

Given a lattice with a basis: $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$

Metric tensor $\boldsymbol{G}$

$$\boldsymbol{G} = \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}^T . \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = \begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{bmatrix} . \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix}$$

$$\boldsymbol{G}_{ik} = (\mathbf{a}_i, \mathbf{a}_k) = a_i a_k \cos\alpha_j$$

Metric tensor ***G is symmetric:*** $\boldsymbol{G}_{ik} = \boldsymbol{G}_{ki}$

Metric tensor $\boldsymbol{G}$ in terms of lattice parameters

$$\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix} \quad \boldsymbol{G} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}$$

EXERCISE (Problem 2.4.5)

Write down the metric tensors of the seven crystal systems in parametric form using the general expressions for their lattice parameters. For each of the cases, express the volume of the unit cell as a function of the lattice parameters.

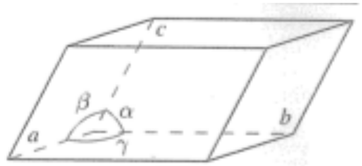
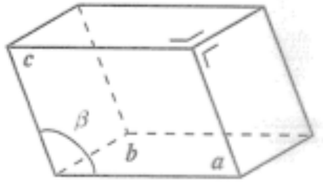
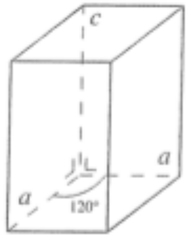
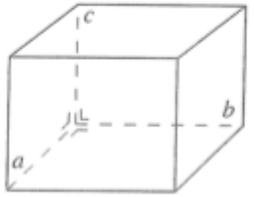
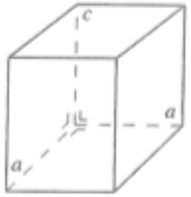
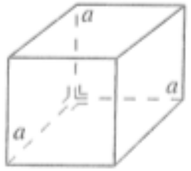
For example:

tetragonal crystal system: $a=b, c, \alpha=\beta=\gamma=90$

$$\boldsymbol{G} = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}$$

V=?

The seven 3D-crystal systems

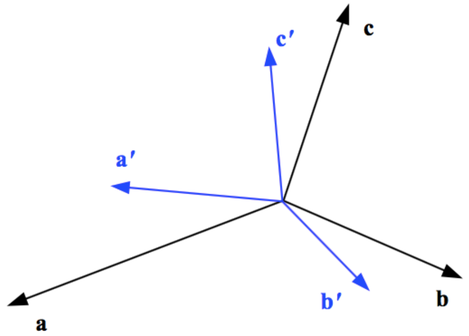
no conditions $\{a, b, c, \alpha, \beta, \gamma\}$	**TRICLINIC (ANORTHIC)**	
$\alpha = \gamma = 90°$† $\{a, b, c, 90, \beta, 90\}$	**MONOCLINIC**	
$a = b$, $\alpha = \beta = 90°$, $\gamma = 120°$ $\{a, a, c, 90, 90, 120\}$	**HEXAGONAL**	
$a = b = c$, $\alpha = \beta = \gamma$ $\{a, a, a, \alpha, \alpha, \alpha\}$	**RHOMBOHEDRAL (TRIGONAL)**	
$\alpha = \beta = \gamma = 90°$ $\{a, b, c, 90, 90, 90\}$	**ORTHORHOMBIC**	
$a = b$, $\alpha = \beta = \gamma = 90°$ $\{a, a, c, 90, 90, 90\}$	**TETRAGONAL**	
$a = b = c$, $\alpha = \beta = \gamma = 90°$ $\{a, a, a, 90, 90, 90\}$	**CUBIC**	

$$\boldsymbol{G} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}$$

$V^2 = \det \boldsymbol{G} =$

$$= a^2 b^2 c^2 (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma).$$

Transformation properties of G under basis transformation



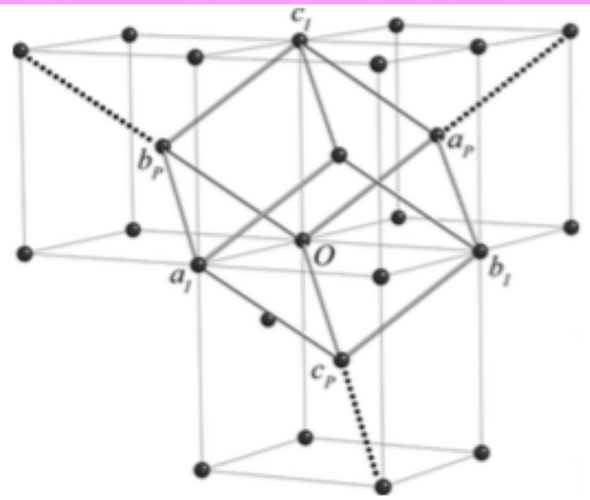
basis transformation:

$$\{\mathbf{a'}_1, \mathbf{a'}_2, \mathbf{a'}_3\} = \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}\, P$$

$$G' = \{\mathbf{a'}_1, \mathbf{a'}_2, \mathbf{a'}_3\}^T . \{\mathbf{a'}_1, \mathbf{a'}_2, \mathbf{a'}_3\} = P^T \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}^T . \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}\, P$$

$$G' = P^T G P$$

Example



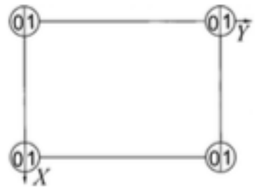
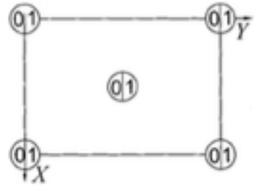
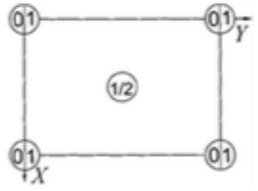
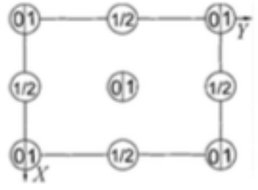
$$P = 1/2 \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

$cI \longrightarrow cP$

$$G_I = a^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad G_P = a^2/4 \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}$$

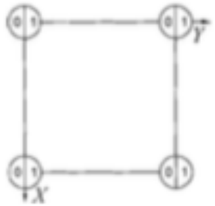
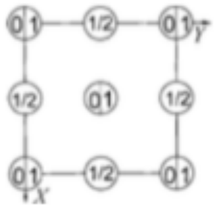
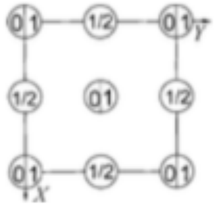
Examples

METRIC TENSORS

Bravais lattice*	Lattice parameters: Conventional	Lattice parameters: Primitive	Metric tensor: Conventional	Metric tensor: Primitive/transf.†	Metric tensor: Relations of the components	Projections
oP	a, b, c $\alpha = \beta = \gamma = 90°$	a, b, c $\alpha = \beta = \gamma = 90°$	$g_{11}\ 0\ 0$ $g_{22}\ 0$ g_{33}			
oC (*oS*)		$a_1 = a_2, c$ $\gamma, \alpha = \beta = 90°$		$\boldsymbol{P}(C)$ $g'_{11}\ g'_{12}\ 0$ $g'_{11}\ 0$ g_{33}	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$	
oI		$a_1 = a_2 = a_3$ α, β, γ $\cos\alpha + \cos\beta + \cos\gamma = -1$		$\boldsymbol{P}(I)$ $-\tilde{g}\ g'_{12}\ g'_{13}$ $-\tilde{g}\ g'_{23}$ $-\tilde{g}$ $\tilde{g} = g'_{12} + g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}(-g_{11} - g_{22} + g_{33})$ $g'_{13} = \frac{1}{4}(-g_{11} + g_{22} - g_{33})$ $g'_{23} = \frac{1}{4}(g_{11} - g_{22} - g_{33})$ $g_{11} = -2(g'_{12} + g'_{13})$ $g_{22} = -2(g'_{12} + g'_{23})$ $g_{33} = -2(g'_{13} + g'_{23})$	
oF		a, b, c α, β, γ $\cos\alpha = \dfrac{-a^2 + b^2 + c^2}{2bc}$ $\cos\beta = \dfrac{a^2 + b^2 + c^2}{2ac}$ $\cos\gamma = \dfrac{a^2 + b^2 - c^2}{2ab}$		$\boldsymbol{P}(F)$ $\tilde{g}_1\ g'_{12}\ g'_{13}$ $\tilde{g}_2\ g'_{23}$ $\tilde{g}_3$ $\tilde{g}_1 = g'_{12} + g'_{13}$ $\tilde{g}_2 = g'_{12} + g'_{23}$ $\tilde{g}_3 = g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}\, g_{33}$ $g'_{13} = \frac{1}{4}\, g_{22}$ $g'_{23} = \frac{1}{4}\, g_{11}$ $g_{11} = 4g'_{23}$ $g_{22} = 4g'_{13}$ $g_{33} = 4g'_{12}$	

Example

METRIC TENSORS

Bravais lattice*	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.†	Relations of the components	
cP	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	g_{11} 0 0 g_{11} 0 g_{11}	g_{11} 0 0 g_{11} 0 g_{11}		
cI	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 109.5°$ $\cos\alpha = -\frac{1}{3}$	g_{11} 0 0 g_{11} 0 g_{11}	***P***(*I*) g'_{11} $-\frac{1}{3}g'_{11}$ $-\frac{1}{3}g'_{11}$ g'_{11} $-\frac{1}{3}g'_{11}$ g'_{11}	$g'_{11} = \frac{3}{4}g_{11}$ $g_{11} = \frac{4}{3}g'_{11}$	
cF	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 60°$	g_{11} 0 0 g_{11} 0 g_{11}	***P***(*F*) g'_{11} $\frac{1}{2}g'_{11}$ $\frac{1}{2}g'_{11}$ g'_{11} $\frac{1}{2}g'_{11}$ g'_{11}	$g'_{11} = \frac{1}{2}g_{11}$ $g_{11} = 2g'_{11}$	

* See footnote to Table 9.1.7.1. Symbols in parentheses are standard symbols, see Table 2.1.2.1.
† $\boldsymbol{P}(C) = \frac{1}{2}(110/\bar{1}10/002), \boldsymbol{P}(I) = \frac{1}{2}(\bar{1}\bar{1}1/1\bar{1}1/11\bar{1}), \boldsymbol{P}(F) = \frac{1}{2}(011/101/110), \boldsymbol{P}(R) = \frac{1}{3}(\bar{1}21/\bar{2}11/111)$.

Crystallographic calculations: Volume of the unit cell

The volume V of the unit cell of a crystal structure, *i.e.* the body containing all points with coordinates $0 \leq x_1, x_2, x_3 < 1$, can be calculated by the formula

$$\det(\boldsymbol{G}) = V^2.$$

In the general case one obtains

$$V^2 = \begin{vmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{vmatrix} =$$

$$= a^2\, b^2\, c^2\, (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma).$$

Volume of the unit cell in terms of lattice parameters (Buerger, 1941)

Basis vectors with respect to Cartesian basis

$$\left.\begin{aligned}\mathbf{a} &= \mathbf{i}a_x + \mathbf{j}a_y + \mathbf{k}a_z,\\ \mathbf{b} &= \mathbf{i}b_x + \mathbf{j}b_y + \mathbf{k}b_z,\\ \mathbf{c} &= \mathbf{i}c_x + \mathbf{j}c_y + \mathbf{k}c_z,\end{aligned}\right\} \longrightarrow V = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}$$

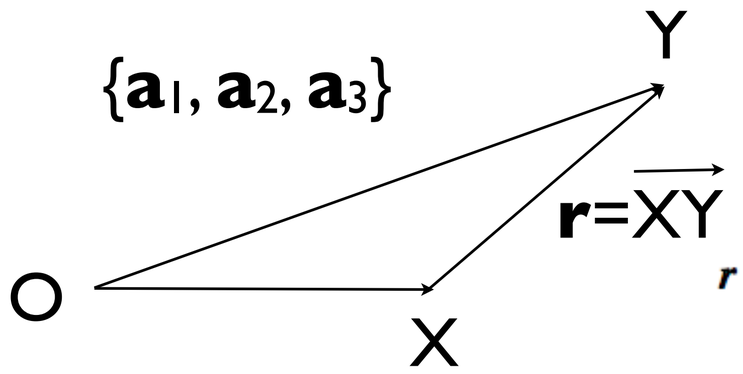
det (A)=det(A^T)

$$V^2 = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} \begin{vmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{vmatrix} = \begin{vmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{vmatrix} = \det(\boldsymbol{G})$$

$$= \begin{vmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ba\cos\gamma & b^2 & bc\cos\alpha \\ ca\cos\beta & cb\cos\alpha & c^2 \end{vmatrix}$$

$$V = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

Crystallographic calculations: Distances or Lengths



$\mathbf{r}=\overrightarrow{XY}=r_1\mathbf{a}_1+r_2\mathbf{a}_2+r_3\mathbf{a}_3,\ r_i\in\mathbb{R}$

$$\boldsymbol{r} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix}, \text{ where } \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \text{ and } \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

length r of r: $r^2=(\mathbf{r},\mathbf{r})=(r_1\mathbf{a}_1+r_2\mathbf{a}_2+r_3\mathbf{a}_3, r_1\mathbf{a}_1+r_2\mathbf{a}_2+r_3\mathbf{a}_3)$

$r^2=(r_1\mathbf{a}_1,r_1\mathbf{a}_1)+(r_2\mathbf{a}_2,r_2\mathbf{a}_2)+(r_3\mathbf{a}_3,r_3\mathbf{a}_3)+2(r_2\mathbf{a}_2,r_3\mathbf{a}_3)+2(r_3\mathbf{a}_3,r_1\mathbf{a}_1)+2(r_1\mathbf{a}_1,r_2\mathbf{a}_2)$

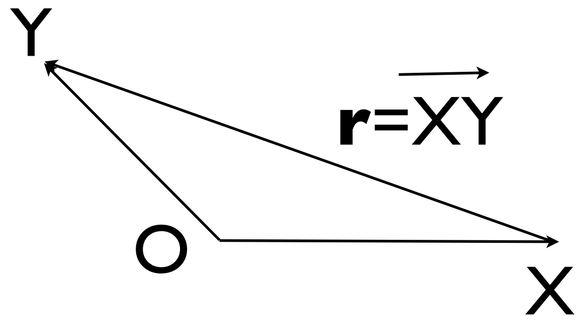
$r^2=r_1^2a_1^2+r_2^2a_2^2+r_3^2a_3^2+2r_2r_3a_2a_3\cos\alpha_1+2r_3r_1a_3a_1\cos\alpha_2+2r_1r_2a_1a_2\cos\alpha_3$

orthonormal basis ($a_1=a_2=a_3=1$, $\alpha_1=\alpha_2=\alpha_3=90$):

$r^2=r_1^2+r_2^2+r_3^2$

Crystallographic calculations: Distances or Lengths

Given a basis:
$\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$



length r of **r**: $r^2=(\mathbf{r},\mathbf{r})$

$$r^2=r_1^2a_1^2+r_2^2a_2^2+r_3^2a_3^2+2r_2r_3a_2a_3\cos\alpha_1+2r_3r_1a_3a_1\cos\alpha_2+2r_1r_2a_1a_2\cos\alpha_3$$

Fundamental matrix (metric tensor)

$\boldsymbol{G}=$

G_{11}	G_{12}	G_{13}
G_{21}	G_{22}	G_{23}
G_{31}	G_{32}	G_{33}

$\boldsymbol{G}_{ik}=(\mathbf{a}_i,\mathbf{a}_k)=a_ia_k\cos\alpha_j,$

$\boldsymbol{G}_{ik}=\boldsymbol{G}_{ki}$

length of a vector:

$r^2=(\mathbf{r}, \mathbf{r})=\mathbf{r}^T\boldsymbol{G}\mathbf{r}$

orthonormal basis

$(a_1=a_2=a_3=1, \alpha_1=\alpha_2=\alpha_3=90)$: $\boldsymbol{G}=\boldsymbol{I}$

$r^2=\mathbf{r}^T\boldsymbol{G}\mathbf{r}=\mathbf{r}^T\mathbf{r}$

Crystallographic calculations: Bonding angle

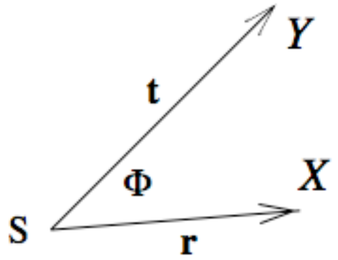


Fig. 1.6.1 The bonding angle Φ between the bond vectors $\overrightarrow{SX} = \mathbf{r}$ and $\overrightarrow{SY} = \mathbf{t}$.

$$(\mathbf{r}\,,\,\mathbf{t}) = |\mathbf{r}|\,|\mathbf{t}|\,\cos\Phi = r\,t\,\cos\Phi,$$

$$r_1\,t_1\,a_1^2 + r_2\,t_2\,a_2^2 + r_3\,t_3\,a_3^2 + (r_2\,t_3 + r_3\,t_2)\,a_2\,a_3\cos\alpha_1 + \\ + (r_3\,t_1 + r_1\,t_3)\,a_1\,a_3\cos\alpha_2 + (r_1\,t_2 + r_2\,t_1)\,a_1\,a_2\cos\alpha_3.$$

$$\cos\Phi = \Big(\sum_{i,k=1}^{3} G_{ik}\,r_i\,r_k\Big)^{-1/2}\Big(\sum_{i,k=1}^{3} G_{ik}\,t_i\,t_k\Big)^{-1/2}\sum_{i,k=1}^{3} G_{ik}\,r_i\,t_k$$

orthonormal basis:

$$r\,t\cos\Phi = r_1\,t_1 + r_2\,t_2 + r_3\,t_3,$$

$$\cos\Phi = \frac{r_1t_1 + r_2t_2 + r_3t_3}{r\,t}$$

Crystallographic calculations: Bonding angle

Given a basis:

$\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$

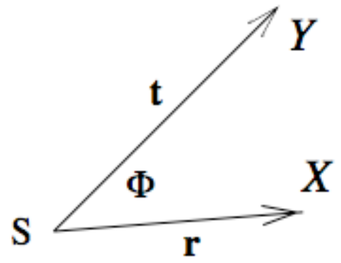


Fig. 1.6.1 The bonding angle Φ between the bond vectors $\overrightarrow{SX} = \mathbf{r}$ and $\overrightarrow{SY} = \mathbf{t}$.

Fundamental matrix (metric tensor)

$\boldsymbol{G}=$

G_{11}	G_{12}	G_{13}
G_{21}	G_{22}	G_{23}
G_{31}	G_{32}	G_{33}

$\boldsymbol{G}_{ik}=(\mathbf{a}_i,\mathbf{a}_k)=a_i a_k \cos\alpha_j,$

$\boldsymbol{G}_{ik}=\boldsymbol{G}_{ki}$

bonding angle:

$$(\mathbf{r}\,,\,\mathbf{t}) = |\mathbf{r}|\,|\mathbf{t}|\,\cos\Phi = r\,t\,\cos\Phi,$$

$(\mathbf{r},\mathbf{t})=\mathbf{r}^{\mathrm{T}}\boldsymbol{G}\mathbf{t}$

$$\cos\Phi = (\boldsymbol{r}^{\mathrm{T}}\,\boldsymbol{G}\,\boldsymbol{r})^{-1/2}\,(\boldsymbol{t}^{\mathrm{T}}\,\boldsymbol{G}\,\boldsymbol{t})^{-1/2}\,\boldsymbol{r}^{\mathrm{T}}\,\boldsymbol{G}\,\boldsymbol{t}.$$