The Brillouin object of the CP-PAW code

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Chapter 1

BRILLOUIN object

1.1 Purpose and theoretical background

The purpose of this object is to perform integrations of matrix elements over the occupied part of Brillouin zone.

$$\langle A \rangle = \sum_n \frac{1}{V_G} \int d^3k \; A_n(\vec{k}) \theta(\epsilon_n(\vec{k}) - \mu) \tag{1.1}$$

where the matrix of the one-particle operator $\hat{A}$ elements are

$$A_n(\vec{k}) = \langle \psi_n(\vec{k}) | \hat{A} | \psi_n(\vec{k}) \rangle \tag{1.2}$$

and $\epsilon_n(\vec{k})$ are the one-particle energies, the eigenvalues of the Hamiltonian.

In the linear tetrahedron method[1, 2, 3], the function values are evaluated at a set of discrete k-points $\vec{k}_j$ and energy levels and matrix elements are linarly interpolated within tetrahedra filling the space between the grid points.

The BRILLOUIN object selects the grid points and reduces them on the basis of point groups symemtry operations of the crystal.

If the integral is performed as linear interpolation between grid points, it can be written in the simple form

$$\langle A \rangle = \sum_n \sum_j w_n(\vec{k}_j) A_n(\vec{k}_j) \tag{1.3}$$

where the integration weights are independent of the type if matrix element to be integrated.[3] They are evaluated using the tetrahedron method.

The integration weights include a quadratic correction, which improves the integrals substantially beyond the purely linear approximation.[3]

1.2 Code structure: Brillouin

1.2.1 Brillouin_module

The object has an internal memory, which is kept in the Brillouin module in the data structure `THIS`.

```
TYPE THIS_TYPE
  INTEGER(4)              :: NKP       ! #(IRREDUCIBLE KPOINTS)
  INTEGER(4)              :: NTET      ! #(IRREDUCIBLE TETRAHEDRA)
  REAL(8)                 :: VOL       ! 1/#(GENERAL TETRAHEDRA)
  REAL(8)                 :: RBAS(3,3) ! REAL SPACE LATTICE VECTORS
  integer(4)              :: NKDIV(3)
  integer(4)              :: ishift(3)
  REAL(8)       ,POINTER :: XK(:,:)   !(3,NKP) IRR. K-POINTS IN RELATIVE COORDINATES
  INTEGER(4)    ,POINTER :: IKP(:,:)  !(4,NTET) TETRAHEDRON CORNERS
  INTEGER(4)    ,POINTER :: MULT(:)   !(NTET) MULTIPLICITY OF THE TETRAHEDRON
  INTEGER(4)    ,POINTER :: irrkp(:)  !(nmshp) pointer to irr. k-point
END TYPE THIS_TYPE
```

1.2.2 Brillouin_msh

- RBAS real-space lattice vectors in kartesian coordinates
- NGKP Target value of the number of general k-points on the interpolation grid
- NSYM number of generators for the point group operations
- IARB
- TSHIFT

First, the k-point grid is defined by determining the division of the lattice vectors $N(3)$ in `brillouin_basdiv`. The value $NMSHPNT = (N(1)+1)*(N(2)+1)*(N(3)+1)$ is returned. The grid divisions are placed onto `this%nkdiv`

In `brillouin_reduz` the k-points are mapped onto each other using the point group operations

$$\vec{k}_{i_1,i_2,i_3} = \sum_{j=1}^{3} \vec{g}_j \frac{i_j + \frac{1}{2}\tau_j}{n_j} \vec{i'} = \boldsymbol{O}\vec{i}$$

In this way a mapping between k-points is established. For two symetry related k-points the mapping always goes to the k-point with the lower value according to some unique numbering scheme.

In `brillouin_zuord` this mapping is used to determine the irreducible k-points on the grid. The irreducible k-points are the those that are mapped under the mapping `NUM` onto themselfes Those k-points will be calculated in relative coordinates as XK an the mapping NUM will be modified so that the general k-points point onto the irreducible k-points in their own arrangement.

The tetrahedra are calculated and mappend onto irreducible ones.

Chapter 2

SPACEGROUP object

2.1 Purpose and theoretical background

2.1.1 Symmetry operations

The symmetry operations can be found in the book by Bradley and Cracknell[4], which lists in table 3.4 *"Results of operatoes on the reciprocal lattice vectors"* the point group operations in terms of reciprocal lattice vectors of all the space-point groups of crystals. Note that the operations in terms of real space lattice vectors differ from those in reciprocal lattice vectors.

It is very important that the real-space lattice vectors are chosen exactly in the convention of table 3.1 *"The 14 Bravais lattices"* of Bradley Cracknell. There are different possible choices, but only the one given in the book is compatible with teh transformations in Table 3.4.

2.1.2 Bravais lattices

The SPACEGROUP object works only with the choice of unit cells used by Bradley and Cracknell[4] in their table

Bravais Lattice		$\vec{T}_1$	$\vec{T}_2$	$\vec{T}_3$
triclinic				
primitive	Γ_1			
monoclinic				
primitive	Γ_m	$(0,-b,0)$	$(a\sin(\gamma),-a\cos(\gamma),0)$	$(0,0,c)$
base centered	Γ_m^b	$(0,-b,0)$	$\frac{1}{2}(a\sin(\gamma),-a\cos(\gamma),-c)$	$\frac{1}{2}(a\sin(\gamma),-a\cos(\gamma),c)$
orthorhombic				
primitive	Γ_o	$(0,-b,0)$	$(a,0,0)$	$(0,0,c)$
base centered	Γ_o^b	$(\frac{1}{2}a,-\frac{1}{2}b,0)$	$(\frac{1}{2}a,\frac{1}{2}b,0)$	$(0,0,c)$
body centered	Γ_o^v	$\frac{1}{2}(a,b,c)$	$\frac{1}{2}(-a,-b,c)$	$\frac{1}{2}(a,-b,-c)$
face centered	Γ_o^f	$\frac{1}{2}(a,0,c)$	$\frac{1}{2}(0,-b,c)$	$\frac{1}{2}(a,-b,0)$
tetragonal				
primitive	Γ_q	$(a,0,0)$	$(0,a,0)$	$(0,0,c)$
body centered	Γ_q^v	$\frac{1}{2}(-a,a,c)$	$\frac{1}{2}(a,-a,c)$	$\frac{1}{2}(a,a,-c)$
trigonal				
primitive	Γ_{rh}	$(0,a,c)$	$(\frac{1}{2}\sqrt{3}a,\frac{1}{2}a,c)$	$(-\frac{1}{2}\sqrt{3}a,\frac{1}{2}a,c)$
hexagonal				
primitive	Γ_h	$(0,-1,0)a$	$(\frac{1}{2}\sqrt{3},\frac{1}{2},0)a$	$(0,0,1)c$
cubic				
primitive	Γ_c	$(1,0,0)a$	$(0,1,0)a$	$(0,0,1)a$
face centered	Γ_c^f	$\frac{1}{2}a(0,1,1)$	$\frac{1}{2}a(1,0,1)$	$\frac{1}{2}a(1,1,0)$
body centered	Γ_c^v	$\frac{1}{2}a(-1,1,1)$	$\frac{1}{2}a(1,-1,1)$	$\frac{1}{2}a(1,1,-1)$

2.1.3 Symmetry operations

Schoenflies symbol	Description
E	identity
I	inversion
C_n	anticlockwise n-fold rotation (proper rotation)
S_n	anticlockwise n-fold rotation followed by a reflection about a plane perpendicular to the rotation axis
$\sigma = C_2 \cdot I$	reflection

- The reflection can be expressed by a two-fold rotation about an axis perpendicular to the mirror plane followed by an inversion.
- The improper rotation $S(\phi)$ can also be expressed as product of a proper rotation $C(\pi+\phi)$

followed by an inversion.

$$C(\phi) = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad S(\phi) = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$I \cdot C(\pi+\phi) = \begin{pmatrix} -\cos(\pi+\phi) & \sin(\pi+\phi) & 0 \\ -\sin(\pi+\phi) & -\cos(\pi+\phi) & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} -\cos(\pi+\phi) & \sin(\pi+\phi) & 0 \\ -\sin(\pi+\phi) & -\cos(\pi+\phi) & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & -1 \end{pmatrix} = S(\phi) \tag{2.1}$$

Thus $S_3^+ = I \cdot C_6^-$, $S_4^+ = I \cdot C_4^-$ and $S_6^+ = I \cdot C_3^-$.

The following list explains all the symmetry elements for all lattice systems, and it contains a list of generators used lateron.

Triclinic system Γ_1
Generators: I, ...

Monoclinic system Γ_m, Γ_m^b					
2-fold rotation	axis				
C_{2z}, σ_z	(1,0,0)				
Generators: I, ...					

Orthorhomic system $\Gamma_o, \Gamma_o^b, \Gamma_o^v, \Gamma_0^f$					
2-fold rotation	axis				
C_{2x}, σ_x	(1,0,0)				
C_{2y}, σ_y	(0,1,0)				
C_{2z}, σ_z	(0,0,1)				
Generators: I, ...					

Tetragonal system Γ_q, Γ_q^v					
2-fold rotation	axis	4-fold rotation	axis		
C_{2x}, σ_x	(1,0,0)	$C_{4z}^{\pm}, S_{4z}^{\mp}$	(0,0,1)		
C_{2y}, σ_y	(0,1,0)				
C_{2z}, σ_z	(0,0,1)				
C_{2a}, σ_a	(?,?,?)				
C_{2b}, σ_b	(?,?,?)				
Generators: I, ...					

Trigonal system Γ_{rh}					
2-fold rotation	axis	3-fold rotation	axis		
C_{21}', σ_{d1}	(?,0,0)	$C_3^{\pm}, S_6^{\mp}$	(?,?,?)		
C_{22}', σ_{d2}	(?,0,0)				
C_{23}', σ_{d3}	(?,0,0)				
Generators: I, ...					

Hexagonal system Γ_h					
2-fold rotation	axis	3-fold rotation	axis	6-fold rotation	axis
C_2, σ_h	(?,?,?)	$C_3^{\pm}, S_6^{\mp}$	(?,?,?)	$C_6^{\pm}, S_3^{\mp}$	(?,?,?)
C_{21}', σ_{d1}	(?,?,?)				
C_{22}', σ_{d2}	(?,?,?)				
C_{23}', σ_{d3}	(?,?,?)				
C_{21}'', σ_{v1}	(?,?,?)				
C_{22}'', σ_{v2}	(?,?,?)				
C_{23}'', σ_{v3}	(?,?,?)				
Generators: I, ...					

Cubic system $\Gamma_c, \Gamma_c^f, \Gamma_c^v$ (see Fig. 1.3 of Bradley Cracknell[4])					
2-fold rotation	axis	3-fold rotation	axis	4-fold rotation	axis
C_{2x}, σ_x	(1,0,0)	C_{31}	(1,1,1)	C_{4x}	(1,0,0)
C_{2y}, σ_y	(0,1,0)	C_{32}	(-1,-1,1)	C_{4y}	(0,1,0)
C_{2z}, σ_z	(0,0,1)	C_{33}	(1,-1,-1)	C_{4z}	(0,0,1)
C_{2a}, σ_a	(1,1,0)	C_{34}	(-1,1,-1)		
C_{2b}, σ_b	(1,-1,0)				
C_{2c}, σ_c	(1,0,1)				
C_{2d}, σ_d	(0,1,1)				
C_{2e}, σ_e	(0,1,1)				
C_{2f}, σ_f	(0,-1,1)				
Generators: $I, C_{2x}, C_{2z}, C_{2a}, \sigma_{da}, C_{31}^+$					

A supersript on the Bravais-lattice symbol Γ means base-centered (b), body-centered (v), face-centered (f). The primitive lattice has no superscript.

All lattice systems can have the identity E and the inversion I as one of its symmetry elements. They are not listed.

2.1.4 Symmetry operations: Table 3.4 of Bradley Cracknell

The transformations are converted into matrices as follows: Let us take the operation C_{32}^+ for the face-centered cubic lattice Γ_c^f:

	Γ_c^f		
C_{32}^+	$-\vec{g}_1 - \vec{g}_2 - \vec{g}_3$	$\vec{g}_1$	$\vec{g}_3$

Table 2.1: Example for an entry of table 3.4 of Bradley Cracknell[4]

The three entries in table 2.1 specify the result of the operation C_{32}^+ onto the first, second, and third lattice vector, that is $\vec{g}_1' = \boldsymbol{U}^{C_{32}^+}\vec{g}_1$, $\vec{g}_2' = \boldsymbol{U}^{C_{32}^+}\vec{g}_2$ and $\vec{g}_3' = \boldsymbol{U}^{C_{32}^+}\vec{g}_3$. Here, $\boldsymbol{U}^{C_{32}^+}$ is the transformation in cartesian coordinates, and $\vec{g}_i$ are the primitive reciprocal lattice vectors in cartesian coordinates.

The transformation C_{32}^+ can be written as sum of dyadic products [1]

$$\boldsymbol{U}^{C_{32}^+} = (-\vec{g}_1 - \vec{g}_2 - \vec{g}_3) \otimes \vec{g}_1 + \vec{g}_1 \otimes \vec{g}_2 + \vec{g}_3 \otimes \vec{g}_3 = \sum_{i,j} O_{i,j}^{\Gamma_c^f, C_{32}^+} \vec{g}_i \otimes \vec{g}_j \tag{2.2}$$

The matrix

$$\boldsymbol{O}^{\Gamma_c^f, C_{32}^+} = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \tag{2.3}$$

[1] Dyadic products (outer products) of two vectors are written as $\vec{a} \otimes \vec{b}$. The resulting matrix gas the elements $(\vec{a} \otimes \vec{b})_{i,j} = a_i b_j$

is the transformation C_{32}^{+} expressed in relative coordinates of the reciprocal lattice vectors $\vec{g}_1, \vec{g}_2, \vec{g}_3$ specified in Table 3.3 of Bradley Cracknell[4] for the face-centered cubic Bravais system Γ_c^f. The matrices $\boldsymbol{O}$ can be obtained directly from table 3.4 of Bradley Cracknell[4].

The meaning of $\boldsymbol{O}^{\Gamma_c^f, C_{32}^{+}}$ as defined in Eq. 2.3 is the following: Under the transformation C_{32}^{+}, the first reciprocal lattice vector $\vec{g}_1$ is transformed onto $\vec{g}_1' = -\vec{g}_1 - \vec{g}_2 - \vec{g}_3$, the second on $\vec{g}_2' = \vec{g}_1$ and that the third vector remains unchanged, i.e. $\vec{g}_3' = \vec{g}_3$.

Note, that the choice made in Table 3.3 of Bradley Cracknell is not unique. The form of the matrix $\boldsymbol{O}^{\Gamma_c^f, C_{32}^{+}}$ relies on the choice of lattice vectors made by Bradley and Cracknell.

The reciprocal lattice vectors can be combined into the matrix $\boldsymbol{g}$. For the example given above, the matrix $\boldsymbol{g}$ has, according to table 3.3, the form

$$\boldsymbol{g}^{\Gamma_c^f} = (\vec{g}_1, \vec{g}_2, \vec{g}_3) = \frac{2\pi}{a} \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \tag{2.4}$$

The matrix $\boldsymbol{g}$ transforms a point $\vec{G}$ in reciprocal space from the relative coordinates $\vec{x}$ into cartesian (absolute) coordinates $\vec{G}$, i.e. $\vec{G} = \boldsymbol{g}\vec{x}$. Thus, a transformation can be written in relative and absolute coordinates as

$$\begin{aligned} \vec{G}' &= \boldsymbol{U}\vec{G} \\ \vec{x}' &= \boldsymbol{O}\vec{x} \end{aligned} \tag{2.5}$$

Thus, the operation $\boldsymbol{U}$ in Cartesian coordinates is obtained from $\boldsymbol{O}$

$$\boldsymbol{U} = \boldsymbol{g}\boldsymbol{O}\boldsymbol{g}^{-1} \tag{2.6}$$

For the specific example, we obtain

$$\begin{aligned} \boldsymbol{U}^{C_{32}^{+}} = \boldsymbol{g}^{\Gamma_c^f} \boldsymbol{O}^{\Gamma_c^f, C_{32}^{+}} \left(\boldsymbol{g}^{\Gamma_c^f}\right)^{-1} &= \underbrace{\frac{2\pi}{a} \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}}_{\boldsymbol{g}} \underbrace{\begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}}_{\boldsymbol{O}} \underbrace{\frac{a}{2\pi} \cdot \frac{1}{2} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}}_{\boldsymbol{g}^{-1}} \\ &= \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \end{aligned} \tag{2.7}$$

The result is a three fold rotation about the axis $(1, 1, -1)$ expressed in cartesian coordinates, while $\boldsymbol{O}^{\Gamma_c^f, C_{32}^{+}}$ is the same operation expressed in relative coordinates for the lattice vectors $\boldsymbol{g}^{\Gamma_c^f}$.

2.1.5 Transformation matrices

Because the Brillouin object transforms the points on the grid, it directly works with relative coordinates $\vec{x}$. A k-point is given as

$$\vec{G}_{i_1, i_2, i_3} = \boldsymbol{g}\vec{x}_{i_1, i_2, i_3} \tag{2.8}$$

where $\vec{x}_{i_1, i_2, i_3} = (\frac{i_1 - 1}{n_1}, \frac{i_2 - 1}{n_2}, \frac{i_3 - 1}{n_3})$ and therefore $\vec{k}_{i_1, i_2, i_3} = \vec{g}_1 \frac{i_1 - 1}{n_1} + \vec{g}_2 \frac{i_2 - 1}{n_2} + \vec{g}_3 \frac{i_3 - 1}{n_3}$. In order to transform the indices (i_1, i_2, i_3), we only need the matrix $\boldsymbol{O}$.

The operations needed by the Brillouin object are these matrices $\boldsymbol{O}$

Convert operations from reciprocal to real space

If the operations $\boldsymbol{O}$ are given for reciprocal space, the ones in real space can be constructed via a transformation into cartesian coordinates.

Let $\boldsymbol{O}$ be the operation relative to the reciprocal lattice vectors $\boldsymbol{g}$, and $\boldsymbol{P}$ the operation relative to the real lattice vectors $\boldsymbol{T}$. We obtain the conversion by

$$\begin{aligned} \boldsymbol{U} &\overset{\text{Eq. 2.6}}{=} \boldsymbol{g}\boldsymbol{O}\boldsymbol{g}^{-1} \\ \boldsymbol{U} &= \boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1} \\ \Rightarrow \boldsymbol{P} &= \boldsymbol{T}^{-1}\boldsymbol{g}\boldsymbol{O}\boldsymbol{g}^{-1}\boldsymbol{T} = \boldsymbol{T}^{-1}\left(2\pi\boldsymbol{T}^{-1,\top}\right)\boldsymbol{O}\left(2\pi\boldsymbol{T}^{-1,\top}\right)^{-1}\boldsymbol{T} \\ &= \boldsymbol{T}^{-1}\boldsymbol{T}^{-1,\top}\boldsymbol{O}\boldsymbol{T}^{\top}\boldsymbol{T} \\ &= \left(\boldsymbol{T}^{\top}\boldsymbol{T}\right)^{-1}\boldsymbol{O}\left(\boldsymbol{T}^{\top}\boldsymbol{T}\right) \end{aligned} \tag{2.9}$$

If the matrix $\boldsymbol{P}$ contains non-integer entries, there is an inconsistency between the operations and the Bravais lattice chosen.

2.1.6 Generators

The point group can be built up from a small number of generators. All operations in a point group can be obtained from the set of generators by multiplying the generators in arbitrary combinations and powers with each other.

The generators for each of the 230 point groups are listed in table 3.7 of Bradley Cracknell. We observe that there are at most five generators for each point group.

2.2 Code structure: Spacegroup

It is important to initialize the spacegroup object by specifying a space group. This is done by giving the space group number using `SPACEGROUP$SETI4('spacegroup',VAL)`. All subsequent operations will refer to this spacegroup only. Changing to a different space group is possible at any time.

The subroutines are

```
SUBROUTINE SPACEGROUP$SETI4(ID,VAL)
SUBROUTINE SPACEGROUP$GETCH(ID,VAL)
SUBROUTINE SPACEGROUP$RBAS(BRAVAIS,A0,B0,C0,ALPHA,BETA,GAMMA,RBAS)
  SUBROUTINE SPACEGROUP$ABCALPHABETAGAMMA(SWITCH,A,B,C,ALPHA,BETA,GAMMA,T)
SUBROUTINE SPACEGROUP$GENERATORS(ID,NOPX,NOP,OPERATION,C)
SUBROUTINE SPACEGROUP$COMPLETE(NOPX,NOP,OP,C)
```

- with `SPACEGROUP$SETI4('SPACEGROUP',val)` one sets the spacegroup by its space group number
- with `SPACEGROUP$GETCH('BRAVAIS',val)` one retrieves the symbol for the corresponding bravais lattice

- with `SPACEGROUP$RBAS` one specifies the lattice vectors by supplying the lattice parameters $a, b, c, \alpha, \beta, \gamma$. Note that angles are given in radian (not degree).
- with `SPACEGROUP$GENERATORS` the generators of the group are obtained either in real or in reciprocal space.
- with `SPACEGROUP$COMPLETE` the set of generators is expanded to the full point group.

2.2.1 SPACEGROUP$GENERATORS

With `ID='REAL'` or `ID='RECI'` one selects the operations in real or reciprocal space. Note that the translations `C` are zero in reciprocal space.

An operation is specified by an integer matrix $\boldsymbol{O}$, which transforms the reciprocal lattice vectors and a vector $\vec{c}$ which defines the transformation of the relative coordinates in real space as

$$\vec{x'} = \boldsymbol{P}\vec{x} + \vec{c} \tag{2.10}$$

The cartesian coordimates are then

$$\vec{r'} = \boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1}\vec{r} + \boldsymbol{T}\vec{c} \tag{2.11}$$

where $\boldsymbol{T}$ is the matrix of real-space lattice vectors.

The real space operation $\boldsymbol{P}$ is obtained from the reciprocal space operation $\boldsymbol{O}$ via Eq. 2.9.

.1 Spacegroups

The translation between the spacegroup number and the international space group symbols is given in tables 2 and 3.

1	P1	2	$P\bar{1}$	3	P2	4	$P2_1$	5	C2
6	Pm	7	Pc	8	Cm	9	Cc	10	P2/m
11	$P2_1/m$	12	C2/m	13	P2/c	14	$P2_1/c$	15	C2/c
16	P222	17	$P222_1$	18	$P2_12_12$	19	$P2_12_12_1$	20	$C222_1$
21	C222	22	F222	23	I222	24	$I2_12_12_1$	25	Pmm2
26	$Pmc2_1$	27	Pcc2	28	Pma2	29	$Pca2_1$	30	Pnc2
31	$Pmn2_1$	32	Pba2	33	$Pna2_1$	34	Pnn2	35	Cmm2
36	$Cmc2_1$	37	Ccc2	38	Amm2	39	Aem2	40	Ama2
41	Aea2	42	Fmm2	43	Fdd2	44	Imm2	45	Iba2
46	Ima2	47	Pmmm	48	Pnnn	49	Pccm	50	Pban
51	Pmma	52	Pnna	53	Pmna	54	Pcca	55	Pbam
56	Pccn	57	Pbcm	58	Pnnm	59	Pmmn	60	Pbcn
61	Pbca	62	Pnma	63	Cmcm	64	Cmce	65	Cmmm
66	Cccm	67	Cmme	68	Ccce	69	Fmmm	70	Fddd
71	Immm	72	Ibam	73	Ibca	74	Imma	75	P4
76	$P4_1$	77	$P4_2$	78	$P4_3$	79	I4	80	$I4_1$
81	$P\bar{4}$	82	$I\bar{4}$	83	P4/m	84	$P4_2/m$	85	P4/n
86	$P4_2/n$	87	I4/m	88	$I4_1/a$	89	P422	90	$P42_12$
91	$P4_122$	92	$P4_12_12$	93	$P4_222$	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	$I\bar{4}c2$

Table 2: Space group number as given in the "International tables for Crystallography, Vol. A" and the corresponding international space group symbol (Herman-Maughin notation). Retrieved from the Bilbao Crystallographic Server http://www.cryst.ehu.es/cryst/text/table.html on Dec. 21, 2013. For further information, see Aroyo, et. al. Zeitschrift für Kristallographie (2006), 221, 1, 15-27.

121	$I\bar{4}2m$	122	$I\bar{4}2d$	123	$P4/mmm$	124	$P4/mcc$	125	$P4/nbm$
126	$P4/nnc$	127	$P4/mbm$	128	$P4/mnc$	129	$P4/nmm$	130	$P4/ncc$
131	$P4_2/mmc$	132	$P4_2/mcm$	133	$P4_2/nbc$	134	$P4_2/nnm$	135	$P4_2/mbc$
136	$P4_2/mnm$	137	$P4_2/nmc$	138	$P4_2/ncm$	139	$I4/mmm$	140	$I4/mcm$
141	$I4_1/amd$	142	$I4_1/acd$	143	$P3$	144	$P3_1$	145	$P3_2$
146	$R3$	147	$P\bar{3}$	148	$R\bar{3}$	149	$P312$	150	$P321$
151	$P3_112$	152	$P3_121$	153	$P3_212$	154	$P3_221$	155	$R32$
156	$P3m1$	157	$P31m$	158	$P3c1$	159	$P31c$	160	$R3m$
161	$R3c$	162	$P\bar{3}1m$	163	$P\bar{3}1c$	164	$P\bar{3}m1$	165	$P\bar{3}c1$
166	$R\bar{3}m$	167	$R\bar{3}c$	168	$P6$	169	$P6_1$	170	$P6_5$
171	$P6_2$	172	$P6_4$	173	$P6_3$	174	$P\bar{6}$	175	$P6/m$
176	$P6_3/m$	177	$P622$	178	$P6_122$	179	$P6_522$	180	$P6_222$
181	$P6_422$	182	$P6_322$	183	$P6mm$	184	$P6cc$	185	$P6_3cm$
186	$P6_3mc$	187	$P\bar{6}m2$	188	$P\bar{6}c2$	189	$P\bar{6}2m$	190	$P\bar{6}2c$
191	$P6/mmm$	192	$P6/mcc$	193	$P6_3/mcm$	194	$P6_3/mmc$	195	$P23$
196	$F23$	197	$I23$	198	$P2_13$	199	$I2_13$	200	$Pm\bar{3}$
201	$Pn\bar{3}$	202	$Fm\bar{3}$	203	$Fd\bar{3}$	204	$Im\bar{3}$	205	$Pa\bar{3}$
206	$Ia\bar{3}$	207	$P432$	208	$P4_232$	209	$F432$	210	$F4_132$
211	$I432$	212	$P4_332$	213	$P4_132$	214	$I4_132$	215	$P\bar{4}3m$
216	$F\bar{4}3m$	217	$I\bar{4}3m$	218	$P\bar{4}3n$	219	$F\bar{4}3c$	220	$I\bar{4}3d$
221	$Pm\bar{3}m$	222	$Pn\bar{3}n$	223	$Pm\bar{3}n$	224	$Pn\bar{3}m$	225	$Fm\bar{3}m$
226	$Fm\bar{3}c$	227	$Fd\bar{3}m$	228	$Fd\bar{3}c$	229	$Im\bar{3}m$	230	$Ia\bar{3}d$

Table 3: Space group number as given in the "International tables for Crystallography, Vol. A" and the corresponding international space group symbol (Herman-Maughin notation). Retrieved from the Bilbao Crystallographic Server http://www.cryst.ehu.es/cryst/text/table.html on Dec. 21, 2013. For further information, see Aroyo, et. al. Zeitschrift für Kristallographie (2006), 221, 1, 15-27.

.2 Paths in the Brillouin zone

The following is from http://en.wikipedia.org/wiki/Brillouin_zone, Dec.22, 2013.

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