Band structure diagram paths based on crystallography

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Abstract

Systematic and automatic calculations of the electronic band structure are a crucial component of computationally driven high-throughput materials screening. An algorithm, for any crystal, to derive a unique description of the crystal structure together with a recommended band path is indispensable for this task. The band structure is typically sampled along a path on or within the Brillouin zone in reciprocal space. Some points in reciprocal space have higher site symmetries and/or have higher constraints than other points regarding the band structure and therefore are likely to be more important than other points. This work categorizes points in reciprocal space according to its symmetry and provides recommended band paths that cover all special wavevector ($\mathbf{k}$-vector) points and lines necessarily and sufficiently. Points in reciprocal space are labeled such that there is no conflict with the crystallographic convention. The $\mathbf{k}$-vector coefficients of labeled points, which are located at Brillouin zone face and

edge centers as well as vertices, are derived based on a primitive cell compatible with the crystallographic convention, including those with axial ratio-dependent coordinates. The definitions and $\mathbf{k}$-vector coefficients of labeled points and recommended band paths in this study will be useful as a common ground when discussing the band structure.

1. Introduction

Electronic band structure diagrams are plots of energy versus wavevector ($\mathbf{k}$-vector) for a number of bands. Applications include visualization of location of band edges and evaluation of effective carrier mass. The band path on which $\mathbf{k}$-vectors are sampled in reciprocal space is generally along line segments on or within the first Brillouin zone (BZ). A collectively exhaustive predetermined list, applicable to any crystal, that contains labels and $\mathbf{k}$-vector coefficients of relevant points in the BZ as well as a recommended band path connecting labeled points would be very useful. This is especially true for high-throughput calculations [1-4] where automatic band path generation is a necessity when the band structure is to be obtained. Making this comprehensive list is a non-trivial task. The topology of the BZ, which is uniquely determined for each crystal, depends on the Bravais lattice and, in some Bravais lattices, also on "axial ratios", which are relations between lattice parameters. One example of a Bravais lattice with an axial ratio-dependent BZ topology is the base-centered tetragonal lattice, where the BZ is an elongated dodecahedron if $c < a$ and a truncated octahedron if $c > a$.

Band paths are chosen as a set of specific line segments connecting distinctive BZ points as well as those connecting a distinctive BZ point to the Γ point. Here, BZ face and edge centers as well as vertices are denoted as "distinctive BZ points" in this study. The BZ boundary gives additional constraints on the band structure because points on a BZ boundary are at equal distance to two lattice points of the reciprocal lattice. As a result, for instance, band gaps form at BZ boundaries in the nearly free electron model [5]. We note that this geometrical constraint on the band structure is not related to what symmetry operations exist in the reciprocal space group, therefore the constraint regarding the BZ boundary is not related to the crystallographic site symmetry in reciprocal space. BZ vertices and edges may become important because multiple BZ boundaries intersect at these positions. The $\mathbf{k}$-vector coefficients of distinctive BZ points depend on the choice of basis vectors, and those of some BZ edge centers and vertices are also dependent on axial ratios. Furthermore, the recommended band path for a given crystal should reflect the symmetry of the crystal. For instance, including two band paths that are symmetrically equivalent is redundant. Points and line segments with high crystallographic symmetries are generally more important than those with low symmetries, thus $\mathbf{k}$-vectors with high symmetries should be preferentially included in the band path.

Setyawan and Curtarolo (SC) [3] provide a collectively exhaustive list of basis vectors of the “standard primitive cell”, definitions and $\mathbf{k}$-vector coefficients of distinctive BZ points, and suggested band paths. This pioneering work provides a unique band path for any crystal, which facilitates inclusion of information on the band structure in databases of materials properties. Moreover, SC identify $\mathbf{k}$-vector coefficients of many distinctive BZ points, including those that are axial ratio-dependent. The definitions in SC are widely used in online databases including aflowlib [3, 6] and the Materials Project [2, 7]. Although the concept of an automatically determined unique band path is a significant advance, there are three major shortcomings in their work, which obliges us to design a new scheme in band path determination. The first is that their standard cell differs from the crystallographic conventional cell in quite a few situations. Part of us recently outlined a computationally friendly algorithm to transform basis vectors of the crystallographic conventional cell to the corresponding SC standard primitive cell [8], which therefore allows use of SC’s definitions of distinctive BZ points and suggested band paths when starting from the crystallographic conventional cell. Secondly, the labels of distinctive BZ points differ in many cases between SC and the crystallographic convention used by Cracknell *et al*. (CDML) [9] and the Bilbao Crystallographic Server (BCS) [10-14]. Finally, the band path in SC is suggested for each Bravais lattice and relevant axial ratio. If the band path is to reflect the symmetry of the crystal, one must consider the reciprocal space group of the crystal (G^*) that is isomorphic to one of the 73 symmorphic group types [10]. Therefore, in principle, band paths should be recommended for all 73 possible G^*; however, the number of types that need explicit treatment can be reduced.

On the other hand, Aroyo *et al*. [10] employs the reciprocal space group approach to organize $\mathbf{k}$-vector data. In a nutshell, the concept of Wyckoff positions in space group types in direct space can be applied to categorize and distinguish the symmetry of

$\mathbf{k}$-vectors in reciprocal space. Most importantly, orbits of $\mathbf{k}$-vectors can be classified into special $\mathbf{k}$-vector points, special $\mathbf{k}$-vector lines, special $\mathbf{k}$-vector planes, and a set of all general $\mathbf{k}$-vectors, where the number of variable parameters of the corresponding Wyckoff position is zero, one, two, and three, respectively.

We propose in this study a collectively exhaustive list of distinctive BZ point labels and their $\mathbf{k}$-vector coefficients as well as recommended band paths that is compatible with crystallographic convention. Time-reversal symmetry is initially assumed, where only centrosymmetric G^* are considered. The analysis is later extended to cases without time-reversal nor inversion symmetry. The recommended band paths in this study are contained on or within the BZ and pass through, at a minimum, all special $\mathbf{k}$-vector points and lines of G^*. Furthermore, the special $\mathbf{k}$-vector points and lines of the reciprocal space group type with the highest symmetry in the Bravais lattice (G_{high}*) must be included in the recommended band path. In addition, every special $\mathbf{k}$-vector point of G_{high}^* that is not connected to a special $\mathbf{k}$-vector line must be connected by a line segment to the Γ point. To be consistent with crystallographic convention, the labels of distinctive BZ points are named according to CDML [9] and the BCS [10-14], if already defined. Labels that must be defined additionally are chosen not to conflict with labels of special $\mathbf{k}$-vector points, lines and planes in CDML and the BCS, and are denoted with even indices in accordance with the BCS.

Use of a standardized definition of distinctive BZ point labels and recommended band paths would ease comparison of results between various studies. Moreover, a crystallographic analysis of the symmetry of band paths would show the difference in importance in line segments in the band path. We wish the data outlined in this article would be useful in discussing the band structure, effective mass, and other properties where symbols of points in reciprocal space must be addressed.

2. Methodology

One key step in this study is to identify $\mathbf{k}$-vector coefficients of distinctive BZ points. The symmetry of a crystal can be described using one of 230 space group types. Assumption of time-reversal symmetry, which means that the band energies at $\mathbf{k}$ and $-\mathbf{k}$ are the same, imposes inversion symmetry as a generator of G^* and thereby reduces the number of G^* that must be considered to 24 [8]. Cases without time-reversal nor inversion symmetry are discussed afterwards. The isomorphism between G^* and a symmorphic space group G_0 allows us to use concepts defined in direct space, most importantly Wyckoff positions, in G^* [10]. Wyckoff positions based on the crystallographic conventional cell are given in the International Tables of Crystallography A (ITA)[15]. The action of G^* on the $\mathbf{k}$-vectors separates them into orbits of symmetry-equivalent $\mathbf{k}$-vectors where each type of $\mathbf{k}$-vector corresponds to a point orbit Wyckoff position of G_0. The concept of "Wyckoff position of a $\mathbf{k}$-vector" is used in this study, which actually means the Wyckoff position in G_0 that corresponds to the $\mathbf{k}$-vector type in G^*. As a result, one can map each of the 230 space group types into one of the 24 centrosymmetric symmorphic space group types G where symmetry of the BZ of a certain space group type is the same for each G. Relevant special $\mathbf{k}$-vector points and lines are identified for each of the 24 G and all BZ topologies with respect to reciprocal basis vectors. Consequently, $\mathbf{k}$-vector coefficients referred to the conventional ITA basis of G_0, or reciprocal "ITA description" basis vectors, are investigated in this work to classify $\mathbf{k}$-vectors according to Wyckoff positions. This means that transformation of reciprocal crystallographic conventional, SC standard conventional, and SC standard primitive basis vectors to reciprocal "ITA description" basis vectors are necessary. The recommended band path is ultimately described using distinctive BZ points where $\mathbf{k}$-vector coefficients are defined with reciprocal primitive basis vectors. Therefore, reciprocal "ITA description" basis vectors must be able to transform to reciprocal crystallographic primitive basis vectors. The relation between reciprocal crystallographic conventional, crystallographic primitive, and "ITA description" basis vectors can be inferred from Aroyo *et al.*[10]

After deriving transformation matrices, the first process in this study is to convert, for all Bravais lattices except triclinic cells that have to be treated differently, distinctive BZ point labels and $\mathbf{k}$-vector coefficients defined using SC standard primitive reciprocal basis in SC [3] to those using "ITA description" reciprocal basis vectors. The next process is to determine labels of distinctive BZ points that are consistent with crystallographic convention in all centrosymmetric G^*, again except for triclinic cells, for each BZ topology with respect to reciprocal basis vectors. The labels of special $\mathbf{k}$-vector points in the BCS [10-14] are compared with those in SC. Labels of special $\mathbf{k}$-vector points in the BCS are adopted when defining labels of distinctive BZ points. Distinctive BZ points that exist in SC but not in the BCS are labeled in this study but the label is not necessarily the same between SC and this work. Finally, the $\mathbf{k}$-vector coefficients based on the crystallographic primitive cell is derived for each distinctive BZ point. In addition, the recommended band path is provided for each Bravais lattice and BZ topology with respect to reciprocal crystallographic primitive basis vectors. The band path depends on the relevant G in some Bravais lattices.

Removing time-reversal symmetry doubles the volume of the irreducible BZ wedge if there is no inversion symmetry. In fact, the additional wedge can be taken as the original wedge inverted though the Γ point. Although labels in the BZ are defined for all 73 symmorphic G^* in the BCS [10-14], we propose sampling of the "inverted" wedge when there is no time-reversal nor inversion symmetry. This would reduce the number of cases necessary to be considered and therefore is easier to implement. Moreover, the "inverted" wedge is identical in shape as the original wedge, thus recognition of the relation between points is facilitated. The BCS assigns a "representation domain", which is a simply connected part of the BZ that contains exactly one reciprocal space vector $\mathbf{k}$-vector of each orbit of $\mathbf{k}$, to each of the 73 reciprocal space groups. However, the wedges sampled in this study in case of no time-reversal nor inversion symmetry are not related to the representation domain. A significant difference is that the wedges are two parts of the BZ that are connected at the Γ point only whereas the represented domain is a simply connected part of the BZ. Therefore, there is no need to define the band path for all 73 reciprocal space group types in this study.

3. Definitions

3.1 Cells and basis vectors

Table 1 shows the definition of basis vectors, basis vector lengths, interaxial angles, and coordinate triplets or $\mathbf{k}$-vector coefficients of various cells considered in this work. Basis vector lengths and interaxial angles are collectively referred to as lattice parameters. Direct space basis vectors are column vectors while reciprocal space basis vectors are row vectors. Any $\mathbf{k}$-vector in reciprocal space $\tilde{\boldsymbol{K}} = \left(\tilde{k}_x, \tilde{k}_y, \tilde{k}_z\right)\left(\tilde{\mathbf{a}}^* / \tilde{\mathbf{b}}^* / \tilde{\mathbf{c}}^*\right)$ can be represented by a row vector of $\mathbf{k}$-vector coefficients $\tilde{\boldsymbol{k}} = \left(\tilde{k}_x, \tilde{k}_y, \tilde{k}_z\right)$ and reciprocal basis vectors $\left(\tilde{\mathbf{a}}^* / \tilde{\mathbf{b}}^* / \tilde{\mathbf{c}}^*\right)$.

The definitions of crystallographic conventional cells as given in Hinuma *et al.* [8] and those of standard conventional cells in SC [3] are summarized below. The crystallographic primitive cell described in detail in Section 3.2 is, in principle, defined using Table 2 of Aroyo *et al.* [10] The "reduced" cell is considered in triclinic cells only and is defined in Section 4.2.4. A generalized metric is assumed, and the first setting that appears in Table A1.4.2.7 of the International Tables of Crystallography B (ITB) [16] is always used as the standard setting in crystallographic conventional cells.

3.1.1 *Cubic, tetragonal, and hexagonal lattice systems*

The crystallographic and SC standard conventional cells are the same, where $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$ in cubic systems, $a = b$ and $\alpha = \beta = \gamma = 90^\circ$ in tetragonal systems, and $a = b$, $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$ in hexagonal cells.

3.1.2 *Rhombohedral lattice system*

The crystallographic conventional cell is defined on a hexagonal lattice with $a = b$, $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$ while the SC standard conventional cell is the primitive cell with $a' = b' = c'$ and $\alpha' = \beta' = \gamma'$.

3.1.3 *Orthorhombic lattice system*

$\alpha = \beta = \gamma = 90^\circ$ and $\alpha' = \beta' = \gamma' = 90^\circ$ always hold. Restrictions on basis vector lengths to obtain a unique definition of the crystallographic conventional cell can be identified based in Table 2.2.6.1 of the ITA [15]. With the exception of side-face centered cells, $a < b$, a shortest, or $a < b < c$ is imposed if the "number of distinct projections" in Table 2.2.6.1 is three, two, or one, respectively. The "number of distinct projections" is the same as the number of different symbols for the space group number in Table A1.4.2.7 of the ITB [16]. For face-centered lattices, $a < b$ always holds in all five space group types and $b < c$ is an additional restriction in *F*222, *Fmmm*, and *Fddd*. For side face-centered space group types, $a < b$ is imposed in the space group types where the "number of distinct projections" in Table 2.2.6.1 is three, namely $C222_1$, *C*222, *Cmm*2, *Ccc*2, *Cmmm*, *Cccm*, *Cnna*, and *Ccca*. Using information on specialized metrics of the Euclidean normalizer to obtain restrictions on basis vector lengths may seem more appealing than using Table 2.2.6.1 of the ITA or Table A1.4.2.7 of the ITB, but then space group types *Ibca* and *Imma* (numbers 73 and 74, respectively) need exceptional treatment (Appendix A) in our procedure. On the other hand, the SC standard conventional cell is always $a' < b' < c'$ if not side-face centered, and *C*-centered and $a' < b'$ if side-face centered.

3.1.4 *Monoclinic lattice system*

The crystallographic conventional cell is the "best" cell by Parthé and Gelato [17] that is always *b*-axis unique, $\beta > 90^\circ$, and *C*-centered if side-face centered. The restriction $a < c$ is imposed for space group types *P*2, $P2_1$, *Pm*, *P*2/*m*, and $P2_1/m$ that do not have *C*-centering nor *c*-glide symmetry. These space group types have "$a = c$ and $90 < \beta < 120^\circ$" as a metric that enhances the symmetry of the Euclidean normalizer (Appendix A). In contrast, the SC standard conventional cell is always *a*-axis unique and $\alpha' < 90^\circ$. The restriction $b' < c'$ is imposed on simple monoclinic lattices and the cell is *C*-centered if side-face centered.

3.1.5 *Triclinic lattice system*

The crystallographic conventional cell is the Niggli reduced cell [18, 19]. The set of basis vector lengths of the reciprocal standard conventional cell, $\{k'_a, k'_b, k'_c\}$, is the same as that of a reciprocal primitive cell that is Niggli-reduced in reciprocal space. The interaxial angles of the reciprocal SC standard conventional cell, $(k'_\alpha, k'_\beta, k'_\gamma)$, are all larger than or smaller than 90° and k'_γ is always the closest to 90°.

3.2 Transformation matrices

A single transformation matrix can be used to transform basis vectors and coordinate triplets in direct space as well as reciprocal basis vectors and $\mathbf{k}$-vector coefficients in reciprocal space. The following transformation matrices are considered in this work. A summary of the relations between various cells is given in Fig. 1. The transformation matrix $\boldsymbol{P}$ that relates basis vectors of the crystallographic conventional and crystallographic primitive cells is defined as

$$(\mathbf{a}_\mathrm{P}, \mathbf{b}_\mathrm{P}, \mathbf{c}_\mathrm{P}) = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}.$$

The coordinate triplets, reciprocal basis vectors, and $\mathbf{k}$-vector coefficients transform as $(x_\mathrm{P}, y_\mathrm{P}, z_\mathrm{P})^T = \boldsymbol{P}^{-1}(x, y, z)^T$, $(\mathbf{a}^*_\mathrm{P} / \mathbf{b}^*_\mathrm{P} / \mathbf{c}^*_\mathrm{P}) = \boldsymbol{P}^{-1}(\mathbf{a}^* / \mathbf{b}^* / \mathbf{c}^*)$, and

$(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z}) = (k_x, k_y, k_z)\boldsymbol{P}$, respectively. The $\mathbf{k}$-vector coefficients of the SC standard conventional and SC standard primitive cells transform as

$$(k'_{\mathrm{P}x}, k'_{\mathrm{P}y}, k'_{\mathrm{P}z}) = (k'_x, k'_y, k'_z)\boldsymbol{P}',$$

those of the crystallographic conventional and SC standard conventional cells as

$$(k'_x, k'_y, k'_z) = (k_x, k_y, k_z)\boldsymbol{S},$$

and those of the reciprocal crystallographic primitive and reciprocal "ITA description" cells as

$$(k_{\mathrm{ITA}x}, k_{\mathrm{ITA}y}, k_{\mathrm{ITA}z}) = (k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z})\boldsymbol{Q}.$$

Transformation of $\mathbf{k}$-vector coefficients between conventional and SC standard primitive cells are used extensively in this work; the relation is

$$(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z}) = (k'_{\mathrm{P}x}, k'_{\mathrm{P}y}, k'_{\mathrm{P}z})(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}')^{-1}.$$

These transformation matrices are defined for all Bravais lattices other than *aP* and are outlined in this section. For *aP* cells, the only transformation matrix to be defined relates reciprocal crystallographic primitive and reciprocal "reduced" $\mathbf{k}$-vector coefficients as

$$(k_{\mathrm{R}x}, k_{\mathrm{R}y}, k_{\mathrm{R}z}) = (k_x, k_y, k_z)\boldsymbol{R},$$

which is discussed in Section 4.2.

The transformation matrix $\boldsymbol{P}'$, which is given in SC [3], is shown in Table 2. The transformation matrix $\boldsymbol{P}$ that transforms crystallographic conventional and primitive cells is defined as in Table 3. The matrices are derived from Table 2 of Aroyo *et al.* [10] with the exceptions of *mC* and *oA*. Details regarding deriving $\boldsymbol{P}$ for *mC* are given in Appendix B. The relations between $\mathbf{k}$-vector coefficients in Table 2 of Aroyo *et al.* [10] imply that the primitive cell of *oC* is $\mathbf{a}_{\mathrm{P}} \cdot \mathbf{c}_{\mathrm{P}} = \mathbf{b}_{\mathrm{P}} \cdot \mathbf{c}_{\mathrm{P}} = 0$ and that of *oA* is

$\mathbf{b}_\mathrm{P}\cdot\mathbf{a}_\mathrm{P}=\mathbf{c}_\mathrm{P}\cdot\mathbf{a}_\mathrm{P}=0$ in their study. However, we define the crystallographic primitive cell of *oA* to be $\mathbf{a}_\mathrm{P}\cdot\mathbf{c}_\mathrm{P}=\mathbf{b}_\mathrm{P}\cdot\mathbf{c}_\mathrm{P}=0$ instead of $\mathbf{b}_\mathrm{P}\cdot\mathbf{a}_\mathrm{P}=\mathbf{c}_\mathrm{P}\cdot\mathbf{a}_\mathrm{P}=0$. The only symmorphic space group type in *oS* where the standard setting is *A*-centered is *Amm*2. However, the standard setting when inversion symmetry is added as a generator to this space group is *Cmmm*, which is also the only *G* in *oS*. Therefore, we choose the crystallographic primitive basis vectors of *oS* to be $\mathbf{a}_\mathrm{P}\cdot\mathbf{c}_\mathrm{P}=\mathbf{b}_\mathrm{P}\cdot\mathbf{c}_\mathrm{P}=0$, which is the natural choice of primitive basis vectors in *Cmmm*, regardless of whether the standard setting of the crystallographic conventional cell is *oC* or *oA*. Subsequently, $\boldsymbol{P}$ for *oA* is derived by first converting the basis of the conventional cell such that the centering is *C*-centered and then applying the relevant matrix for *oC*. Defining the basis vectors of the crystallographic conventional cell for *oC* as $(\mathbf{a}_\mathrm{C},\mathbf{b}_\mathrm{C},\mathbf{c}_\mathrm{C})$ and for *oA* as $(\mathbf{a}_\mathrm{A},\mathbf{b}_\mathrm{A},\mathbf{c}_\mathrm{A})$,

$$(\mathbf{a}_\mathrm{C},\mathbf{b}_\mathrm{C},\mathbf{c}_\mathrm{C})=(\mathbf{a}_\mathrm{A},\mathbf{b}_\mathrm{A},\mathbf{c}_\mathrm{A})\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}.$$

Therefore, for *oA*,

$$\boldsymbol{P}=\frac{1}{2}\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}\begin{pmatrix}1&1&0\\\bar{1}&1&0\\0&0&2\end{pmatrix}=\frac{1}{2}\begin{pmatrix}0&0&2\\1&1&0\\\bar{1}&1&0\end{pmatrix}.$$

The transformation matrix $\boldsymbol{S}$ that transforms crystallographic and standard conventional cells is derived in Hinuma *et al.* [8] and shown in Table 4. $\boldsymbol{S}$ is necessary in this work to convert $\mathbf{k}$-vector coefficients of distinctive BZ points labeled in SC to those in a reciprocal crystallographic cell. One set of labels of distinctive BZ points for each BZ topology with respect to reciprocal crystallographic primitive basis vectors is to be defined in every centrosymmetric G^*. The original label of distinctive BZ points in SC [3] has no relation to the final label of distinctive BZ points tabulated in this study. Therefore, only one among multiple $\boldsymbol{S}$ that results in the same BZ topology with respect to standard primitive basis vectors is given, which is the case in *oP*, *oI*, *oF* when a^{-2},b^{-2},c^{-2} can be edges of a triangle, and *mP*. Note that $b^{-2}>a^{-2}+c^{-2}$ never appears as a condition in *oF* because $a<b$ always hold. The transformation matrix $\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'$ is summarized in Table 5. The transformation matrix

$\boldsymbol{Q}$ given in Table 6 is derived, in principle, from Tables 2 and 3 of Aroyo *et al*. [10] and Table 1.5.4.2 of the ITB [16]. The transformation matrix for *mC* cannot be directly obtained from Tables 2 and 3 of Aroyo *et al*. [10] for the reason described in Appendix B.

4. Derivation of the recommended band path

The goal of this study is to provide labels and $\mathbf{k}$-vector coefficients of distinctive BZ points as well as to propose a recommended band path in drawing a band structure diagram. Information on tables and figures relevant to each Bravais lattice is summarized in Table 7. Ideally one would solely use data regarding distinctive BZ points in CDML [9] and the BCS [10-14]. However, explicit description of $\mathbf{k}$-vector coefficients of some crucial distinctive BZ points, such $\mathbf{k}$-vector coefficients of axial ratio-dependent distinctive BZ points, are not available in the BCS. In contrast, SC [3] provide information on labels and $\mathbf{k}$-vector coefficients of distinctive BZ points for each Bravais lattice and BZ topology, but these are based on their SC standard primitive cells, not on cells based on crystallographic convention. Nevertheless, the information on coordinates of axial ratio-dependent $\mathbf{k}$-vector coefficients of distinctive BZ points in SC is valuable in deriving those based on the crystallographic primitive cell ("reduced" cell in *aP*). Therefore, the first step is to convert $\mathbf{k}$-vector coefficients of distinctive BZ points in SC to a basis compatible with crystallographic convention, that is, the "ITA description" basis in this study. The labels in SC are not inherited in the list of labels of distinctive BZ points that would be tabulated in this work.

The second step is to compare information on distinctive BZ points between the BCS [10-14] and SC [3] for all centrosymmetric G^* and BZ topology with respect to reciprocal basis vectors. The recommended band path in this study must contain, at a minimum, one orbit representative of every special $\mathbf{k}$-vector point and special $\mathbf{k}$-vector line. Aroyo *et al*. [10] defines two $\mathbf{k}$-vectors to be uni-arm if these are related by parameter variation, and "the description of $\mathbf{k}$-vector stars of a Wyckoff position is called uni-arm if the $\mathbf{k}$-vectors representing these stars are uni-arm". This uni-arm description is not always convenient in this work because the uni-arm description of a special $\mathbf{k}$-vector line may protrude from the BZ. In this case, orbit representatives of the special $\mathbf{k}$-vector line are separated into two line segments where both ends of these line segments are distinctive BZ points.

The final step is to transform $\mathbf{k}$-vector coefficients from the reciprocal "ITA description" cell to the reciprocal conventional primitive cell. This is done for each Bravais lattice and BZ topology with respect to reciprocal basis vectors. Furthermore, the recommended band path is given, which includes orbit representatives of all special $\mathbf{k}$-vector lines of G_{high}*. However, orbit splitting of special $\mathbf{k}$-vector lines could happen with symmetry reduction within the same Bravais lattice. Should this situation arise, an additional line segment is added to the recommended band path such that all orbit representatives from special $\mathbf{k}$-vector lines of the low symmetry space group type are included in the band path.

As a final note, when there is no time-reversal nor inversion symmetry, we propose sampling of the additional wedge that is the original irreducible BZ wedge inverted though the Γ point. Labels of distinctive BZ points in the "inverted" wedge are denoted with primes of the original wedge, and the additional recommended band path is the original band path that is inverted though the Γ point. In other words, the length of the recommended band path is doubled when there is no time-reversal symmetry. An example is given in Section 4.4.

4.1 Standard to "ITA description"

The goal of this section is to convert $\mathbf{k}$-vector coefficient information on distinctive BZ points defined in SC [3] to a form where its "Wyckoff position" can be readily identified. In other words, the $\mathbf{k}$-vector coefficients must be transformed from those defined with reciprocal standard primitive basis vectors to the reciprocal "ITA description" basis vectors. Tables 8-29 are lists of $\mathbf{k}$-vector coefficient transformation between reciprocal SC standard primitive, crystallographic primitive, and "ITA description" cells. The relations $\left(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{Pz}}\right) = \left(k'_{\mathrm{P}x}, k'_{\mathrm{P}y}, k'_{\mathrm{Pz}}\right)\left(\boldsymbol{P}^{-1}\boldsymbol{SP}'\right)^{-1}$ and $\left(k_{\mathrm{ITA}x}, k_{\mathrm{ITA}y}, k_{\mathrm{ITAz}}\right) = \left(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{Pz}}\right)\boldsymbol{Q}$ are used. Matrices $\left(\boldsymbol{P}^{-1}\boldsymbol{SP}'\right)^{-1}$ and $\boldsymbol{Q}$ as well as definitions of axial ratio-dependent variables are provided in these tables. Triclinic lattices require separate treatment, and therefore no table is provided.

4.2 Special **k**-vector points and lines

If time-reversal symmetry is enforced, G^* is isomorphic to one of the 24 centrosymmetric symmorphic space group types, that is, G_0. Table 30 shows the relevant centrosymmetric symmorphic space group G for each direct space group number and centering. As an example, consider a crystal with space group type $Pna2_1$ (number 33). The relevant symmorphic space group type, where improper symmetry elements are replaced by proper ones, is $Pmm2$ (number 25). Addition of inversion symmetry makes the space group type $Pmmm$ (number 47), which is G. The special **k**-vector points and lines in reciprocal space are directly related to the Wyckoff positions of G_0. As band paths must be contained on or within the BZ in this study, a list of special **k**-vector point and line representatives on or within the BZ must be compiled for all of the 24 centrosymmetric G and BZ topologies with respect to reciprocal basis vectors. Tables 31-64 shows relations between Wyckoff positions, labels in the BCS [10-14] and SC [3], the **k**-vector coefficients in the reciprocal "ITA description" basis, and the range of special **k**-vector lines. Representatives of all special **k**-vector points and lines as well as distinctive BZ points defined in SC are listed. Special **k**-vector lines are not labeled in the final output of this study but are described by distinctive BZ point labels on each end of a special **k**-vector line segment. Multiple segments may be necessary to contain all orbit representatives, and such cases are expressed, for instance, as $32f$=(Γ-P)+(P-H) for $G = Im\bar{3}m$ (Table 35, $G^* = (Fm\bar{3}m)^*$, $G_0 = Fm\bar{3}m$). Wyckoff positions denoted in round brackets and square brackets correspond to special **k**-vector planes and to the general position, respectively. The following are comments regarding specific Bravais lattices.

4.2.1 *cP*

The label "X_1" denotes a point even though the index is odd. A number of points with odd indices are defined for cubic lattices in the BCS [10-14], and this point is one of them.

4.2.2 *oI*

The unique G for *oI* is *Immm*. The BCS provides BZ labels and **k**-vector coefficients for when b is largest or c is largest. As there are *oI* space group types where use of the standard setting may result in a becoming the longest basis vector (*Ima*2 and *Imma*, numbers 46 and 74, respectively), we also provide data for when a is the largest.

4.2.3 *mC*

Some special $\mathbf{k}$-vector points and lines defined in the BCS [10-14] are not contained within the BZ. These points are labeled as (ex), and another representative on or within the BZ is defined. A parallelepiped primitive cell is provided instead of the BZ for *mP*, *mC*, and *aP* in CDML [9]. Therefore, there is no information on distinctive BZ points that are not at the surface of the parallelepiped in the BCS.

4.2.4 *aP*

As in *mC* (section 4.2.3), some special $\mathbf{k}$-vector points and lines defined in the BCS [10-14] are not contained on or within the BZ, therefore are treated similarly. Analysis starting from the "reduced" cell rather than the crystallographic conventional cell is appropriate in *aP* cells. The "reduced" cell is defined in this study such that the set of reciprocal basis vector lengths, $\{k_{\mathrm{R}a}, k_{\mathrm{R}b}, k_{\mathrm{R}c}\}$, is the same as $\{k'_a, k'_b, k'_c\}$. Moreover, the reciprocal interaxial angles $(k_{\mathrm{R}\alpha}, k_{\mathrm{R}\beta}, k_{\mathrm{R}\gamma})$ are all larger than or smaller than 90°, and $|k_{\mathrm{R}a} k_{\mathrm{R}b} \cos k_{\mathrm{R}\gamma}|$ is the smallest among the set $\{|k_{\mathrm{R}b} k_{\mathrm{R}c} \cos k_{\mathrm{R}\alpha}|, |k_{\mathrm{R}c} k_{\mathrm{R}a} \cos k_{\mathrm{R}\beta}|, |k_{\mathrm{R}a} k_{\mathrm{R}b} \cos k_{\mathrm{R}\gamma}|\}$. The "reduced" cell is convenient because the unique reciprocal basis vector that penetrates a parallelogram face when reciprocal interaxial angles are all-acute is always $\mathbf{c}^*_{\mathrm{R}}$ (see Appendix C).

The crystallographic conventional cell, which is also primitive, is Niggli-reduced in direct space. On the other hand, the SC standard conventional and "reduced" cells have a set of reciprocal basis vector lengths that is identical to the cell that is Niggli-reduced in reciprocal space. In consequence, the transformation matrix to convert crystallographic conventional cells to the SC standard conventional or "reduced" cell cannot be described in a simple form. The idea in this study is to use the same label between reciprocal "ITA description" and "reduced" cells if the $\mathbf{k}$-vector coefficients are the same. The following is a procedure to obtain the "reduced" cell. We start with a primitive cell that is Niggli-reduced in reciprocal space; the basis vectors, basis vector lengths, and reciprocal interaxial angles are denoted as $(\mathbf{a}'', \mathbf{b}'', \mathbf{c}'')$, (k''_a, k''_b, k''_c) and $(k''_\alpha, k''_\beta, k''_\gamma)$, respectively. Unfortunately, the transformation matrix from a conventional cell to the Niggli reduced cell cannot be provided in a simple form, although a robust algorithm to derive the Niggli reduced cell exists [18, 19]. The first step is to transform basis vectors into intermediate basis vectors $(\mathbf{a}''', \mathbf{b}''', \mathbf{c}''')$ with (k_a''', k_b''', k_c''') and $(k_\alpha''', k_\beta''', k_\gamma''')$, respectively, such that the set of reciprocal basis vector lengths is conserved and $|k_a''' k_b''' \cos k_\gamma'''|$ is the smallest in the set $\{|k_b''' k_c''' \cos k_\alpha'''|, |k_c''' k_a''' \cos k_\beta'''|, |k_a''' k_b''' \cos k_\gamma'''|\}$. The transformation matrix $\boldsymbol{M}''$ relating $(\mathbf{a}'', \mathbf{b}'', \mathbf{c}'')$ and intermediate basis vectors $(\mathbf{a}''', \mathbf{b}''', \mathbf{c}''')$ is

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

and shown in Table 65. The second step makes the reciprocal interaxial angles all-obtuse or all-acute while conserving the set of basis vector lengths and keeping $|k_{\mathrm{R}a} k_{\mathrm{R}b} \cos k_{\mathrm{R}\gamma}|$ the smallest among $\{|k_{\mathrm{R}b} k_{\mathrm{R}c} \cos k_{\mathrm{R}\alpha}|, |k_{\mathrm{R}c} k_{\mathrm{R}a} \cos k_{\mathrm{R}\beta}|, |k_{\mathrm{R}a} k_{\mathrm{R}b} \cos k_{\mathrm{R}\gamma}|\}$. The transformation matrix $\boldsymbol{M}'''$ relating $(\mathbf{a}''', \mathbf{b}''', \mathbf{c}''')$ to $(\mathbf{a}_\mathrm{R}, \mathbf{b}_\mathrm{R}, \mathbf{c}_\mathrm{R})$ is

$$(\mathbf{a}_\mathrm{R}, \mathbf{b}_\mathrm{R}, \mathbf{c}_\mathrm{R}) = (\mathbf{a}''', \mathbf{b}''', \mathbf{c}''')\boldsymbol{M}'''$$

and shown in Table 66. We use the same symbol between the ITA and the "reduced" cell for the same $\mathbf{k}$-vector coefficients. Some points labeled in the BCS [10-14] are outside the BZ when the reciprocal interaxial angles are all-acute. In this situation, a point in the BZ that is equivalent after translation by a lattice vector is labeled. Tables 67 and 68 shows relations between labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space for *aP*.

4.3. Recommended band path

There are an infinite number of choices of the band path to be used in describing the band structure. We may be only interested in the band structure along a certain line segment or around a certain point in reciprocal space, for instance band maxima or minima. In such cases, band paths should be chosen on a case-by-case basis. However, automatic generation of a certain band path that gives a sufficient overview of the band structure of a given crystal is desirable, especially in high-throughput calculations [1-3]

[4]. This motivates us to determine a recommended band path for each Bravais lattice based on a number of predetermined principles as outlined below. Considering G_{high}^*,

Rule 1: Representatives of all special $\mathbf{k}$-vector points and lines must be included in the band path.

Rule 2: If a BZ face center special $\mathbf{k}$-vector point is not connected to the Γ point by a special $\mathbf{k}$-vector line, the line segment from the special $\mathbf{k}$-vector point to the Γ point is included in the band path.

Rule 3: If a BZ edge center special $\mathbf{k}$-vector point is the terminus of only one special $\mathbf{k}$-vector line, if possible, a band path line segment from the special $\mathbf{k}$-vector point to a BZ vertex or face center special $\mathbf{k}$-vector point is added.

In addition,

Rule 4: All special $\mathbf{k}$-vector points and lines of G^* of the crystal must be included in the band path.

Tables 69-92 are lists of $\mathbf{k}$-vector coefficients of distinctive BZ points based on the reciprocal "ITA description" and conventional primitive basis vectors ("reduced" cell for *aP*). Figs. 2-25 are figures of the BZ, positions of distinctive BZ points, and the recommended band path. One representative each of all special $\mathbf{k}$-vector points is shown as a filled circle, and other distinctive BZ points are shown as empty circles. Line segments of the recommended band path as based on Rules 1-4 are drawn in red, orange, purple, and dotted red lines, respectively. The set of line segments to be sampled is determined from symmetry although there is ambiguity on the order of line segments to be sampled in the band path or the choice among symmetrically equivalent line segments. Representatives from special $\mathbf{k}$-vector lines that are forced to split into two line segments due to geometrical constraints are placed as adjacent line segments in the recommended band path. Orbit splitting of special $\mathbf{k}$-vector lines happens with symmetry reduction in *cP*, *cF*, and *hP* lattices, which forces inclusion of an additional line segment in the recommended band path according to Rule 4 in some space group types, as discussed below.

4.3.1 *cP*

M-X_2 is an additional segment required when G is $Pm\bar{3}$, which corresponds to space group types $P23$, $P2_13$, $Pm\bar{3}$, $Pn\bar{3}$, and $Pa\bar{3}$ (numbers 195, 198, 200, 201, and

205, respectively). Fig. 26 shows calculated band diagrams of Cr_3Si and AlPt for band path X-M-X_2. The Perdew-Burke-Ernzerhof functional [20] based on the generalized gradient approximation is used in conjunction with the projector augmented-wave method [21] as implemented in the VASP code [22-25]. The space group types of these compounds are $Pm\bar{3}n$ and $P2_13$ (numbers 223 and 198), respectively. We find that X-M and M-X_2 are identical in Cr_3Si but not in AlPt, which demonstrates that the recommended band path would depend on the space group type in *cP*.

4.3.2 *cF*

K and U are equivalent points. X-W_1 is an additional segment required when G is $Fm\bar{3}$, which corresponds to space group types $F23$, $Fm\bar{3}$, and $Fd\bar{3}$ (numbers 196, 202, and 203. respectively). The additional band path from distinctive BZ point K can be drawn to either L or W. The line segment from K to W is adopted because K-W is a special $\mathbf{k}$-vector line while K-L is not when G is $Fm\bar{3}$, that is, G^* is $(Im\bar{3})^*$. Both are special $\mathbf{k}$-vector lines when G is $Fm\bar{3}m$, that is, G^* is $(Im\bar{3}m)^*$.

4.3.3 *hP*

K-H_2 is an additional segment required when G is $P\bar{3}1m$, which corresponds to space group types $P312$, $P3_112$, $P3_212$, $P31m$, $P31c$, $P\bar{3}1m$, and $P\bar{3}1c$ (numbers 149, 151, 153, 157, 159, 162, and 163, respectively) or $P\bar{3}$, which corresponds to space group types $P3$, $P3_1$, $P3_2$, and $P\bar{3}$ (numbers 143, 144, 145, and 147, respectively).

4.4. Band path without time-reversal nor inversion symmetry

We propose a procedure to define distinctive BZ points and recommend a band path when there is no time-reversal nor inversion symmetry. Here, *mP* is used as an example. First, we obtain the distinctive BZ point labels and recommended band path when there is time-reversal symmetry (Fig. 20, Table 87). The additional part of the BZ to be sampled when there is no time-reversal nor inversion symmetry is the irreducible BZ wedge when there is time-reversal symmetry that is inverted through the Γ point. Primes are added to BZ points that are inverted. For instance, $(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z})$ of Z is $(0, 1/2, 0)$, hence that of Z' is $(0, -1/2, 0)$. The $(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z})$ of B is $(0, 0, 1/2)$, thus that of B' is

$(0,0,-1/2)$. *B'* is equivalent to B_2, but this point is labeled *B'* to be consistent with other labeled points. The recommended path with time-reversal symmetry is Γ–*Z*–*D*–*B*–Γ–*A*–*E*–*Z*–C_2–Y_2–Γ, and the additional path when there is no time-reversal symmetry is Γ–*Z'*–*D'*–*B'*–Γ–*A'*–*E'*–*Z'*–C_2'–Y_2'–Γ.

5. Summary

A set of recommended band paths is proposed where the line segments on the band path reflect the symmetry of the crystal and the labels of points in reciprocal space are consistent with crystallographic convention [9-14]. The crystallographic primitive cell is defined by applying the transformation matrices in Table 3 to the crystallographic conventional cell defined in Sec. 3.1. The "reduced" cell defined in Sec. 4.2.4 is used instead of the crystallographic cell to derive the $\mathbf{k}$-vector coefficients of triclinic cells. The $\mathbf{k}$-vector coefficients of distinctive BZ points are defined in Tables 69-92, and figures of the BZ together with the recommended band path are provided in Figs. 2-25. When there is no time-reversal nor inversion symmetry, we propose additional sampling of the irreducible BZ wedge under time-reversal symmetry that is inverted through the Γ point. We wish the definitions and $\mathbf{k}$-vector coefficients of distinctive BZ points and recommended band paths in this study will be used conveniently as a common ground when discussing the band structure.

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Appendix A. The Euclidean normalizer and restrictions on basis vector choice.

The restrictions on basis vector lengths in a conventional cell based on a particular setting is closely related to existence of specialized metrics that result in enhanced symmetry in the Euclidean normalizer. The Euclidean normalizer for monoclinic and orthorhombic lattices is outlined in Table 15.2.1.3 of the ITA [15]. One example of a specialized metric that enhances symmetry of the Euclidean normalizer is $a = b$ in space group type *Cmm*2; the Euclidean normalizer in the general metric ($a \neq b$) is *Pmmm* while that of the enhanced metric ($a = b$) is *P*4/*mmm*.

For monoclinic cells, the restriction $a < c$ is imposed to obtain a unique conventional cell under the standard setting in space group types where "$a = c$ and $90 < \beta < 120^\circ$" is a metric that enhances the symmetry of the Euclidean normalizer. We find that the index of the Euclidean normalizer $N_E(G)$ of the space group *G* doubles under the specialized metric "$a = c$ and $90 < \beta < 120^\circ$" compared to the general metric.

Next, we focus on orthorhombic cells. Here, the Euclidean normalizer of the highest symmetry metric coincides with the affine normalizer $N_A(G)$.[15] Defining *m* as the index of $N_A(G)$ divided by that of $N_E(G)$, and *n* as the number of distinct projections in Table 2.2.6.1 of the ITA, $m \cdot n = 6$ holds except for space group types *Ibca* and *Imma* (numbers 73 and 74, respectively) where $m \cdot n = 12$. Except for these two exceptions, the general metric is $a \neq b$, "$a \neq b$ or $b \neq c$ or $c \neq a$", and $a \neq b \neq c \neq a$ when m is two, three, or six, respectively. These general metrics translate to restrictions $a < b$, "*a* shortest", and $a < b < c$, respectively. In contrast, $a \neq b \neq c \neq a$ and $a \neq b$ is the general metric in space group type *Ibca* and *Imma* but the restriction is *a* shortest and none, respectively. In consequence, although the Euclidean normalizer approach to use *m* in finding restrictions in basis vector lengths of a unique choice of the conventional cell appears elegant, there are exceptions in the procedure that we adopt and therefore the projection approach is more straightforward in orthorhombic cells.

Appendix B. Transformation matrices in *mC*.

Descriptions of **k**-vector types of base-centered monoclinic space groups in CDML [9] are given only in the *c*-axis unique and *A*-centered setting. Therefore, the conversion between $\mathbf{k}$-vector coefficients in the primitive, conventional, and "ITA description" bases should be done based on *mA* not *mC*. Subsequently, transformation of k-vector coefficients in *mC* must be done by first converting to *mA*, transforming using the matrix for *mA* in Table 2 of Aroyo *et al*. [10], and finally converting back to *mC*. Basis vectors, coordinate triplets, and $\mathbf{k}$-vector coefficients in the *b*-axis unique *C*-centered and *c*-axis unique *A*-centered settings are denoted using subscript C and A, respectively. The transformation matrix defined as

$$\boldsymbol{M} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

is used in this Appendix. The relation between the two settings are, according to the ITA, $(\mathbf{a}_\mathrm{C}, \mathbf{b}_\mathrm{C}, \mathbf{c}_\mathrm{C}) = (\mathbf{a}_\mathrm{A}, \mathbf{b}_\mathrm{A}, \mathbf{c}_\mathrm{A})\boldsymbol{M}$. The A and C indices correspond to *mA* and *mC* settings. The $\mathbf{k}$-vector coefficients transform as $(k_{x,\mathrm{C}}, k_{y,\mathrm{C}}, k_{z,\mathrm{C}}) = (k_{x,\mathrm{A}}, k_{y,\mathrm{A}}, k_{z,\mathrm{A}})\boldsymbol{M}$, $(k_{\mathrm{P}x,\mathrm{C}}, k_{\mathrm{P}y,\mathrm{C}}, k_{\mathrm{P}z,\mathrm{C}}) = (k_{\mathrm{P}x,\mathrm{A}}, k_{\mathrm{P}y,\mathrm{A}}, k_{\mathrm{P}z,\mathrm{A}})\boldsymbol{M}$, and $(k_{\mathrm{ITA}x,\mathrm{C}}, k_{\mathrm{ITA}y,\mathrm{C}}, k_{\mathrm{ITA}z,\mathrm{C}}) = (k_{\mathrm{ITA}x,\mathrm{A}}, k_{\mathrm{ITA}y,\mathrm{A}}, k_{\mathrm{ITA}z,\mathrm{A}})\boldsymbol{M}$. According to Tables 2 and 4 of Aroyo *et al*. [10],

$$(k_{x,\mathrm{A}}, k_{y,\mathrm{A}}, k_{z,\mathrm{A}}) = (k_{\mathrm{P}x,\mathrm{A}}, k_{\mathrm{P}y,\mathrm{A}}, k_{\mathrm{P}z,\mathrm{A}})\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$$

and

$$(k_{x,\mathrm{A}}, k_{y,\mathrm{A}}, k_{z,\mathrm{A}}) = (k_{\mathrm{ITA}x,\mathrm{A}}, k_{\mathrm{ITA}y,\mathrm{A}}, k_{\mathrm{ITA}z,\mathrm{A}})\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

In summary, we obtain

$$\boldsymbol{P} = \frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

for *mC*.

Appendix C. BZ face centers in *aP*

The condition that determines the reciprocal standard basis vector of an all-acute triclinic cell, $\mathbf{a}'^*$, $\mathbf{b}'^*$, and $\mathbf{c}'^*$ that penetrates a parallelogram at the BZ surface is derived. Appendix C of Hinuma *et al.*[8] shows that the BZ of a triclinic lattice is a truncated octahedron with 14 faces, and application of the lemma in Appendix B of Hinuma *et al.*[8] shows that $\mathbf{a}'^*/2$, $\mathbf{b}'^*/2$, $\mathbf{c}'^*/2$, $(\mathbf{a}'^* - \mathbf{b}'^*)/2$, $(\mathbf{b}'^* - \mathbf{c}'^*)/2$, $(\mathbf{c}'^* - \mathbf{a}'^*)/2$ and these negatives are always centers of faces. Geometrical analysis shows that exactly one of the following three situations must happen:

1) $\mathbf{a}'^*$ penetrates a parallelogram and $(-\mathbf{a}'^* + \mathbf{b}'^* + \mathbf{c}'^*)/2$ and its negative are centers of the remaining two parallelogram faces.

2) $\mathbf{b}'^*$ penetrates a parallelogram and $(\mathbf{a}'^* - \mathbf{b}'^* + \mathbf{c}'^*)/2$ and its negative are centers of parallelogram faces.

3) $\mathbf{c}'^*$ penetrates a parallelogram and $(\mathbf{a}'^* + \mathbf{b}'^* - \mathbf{c}'^*)/2$ and its negative are centers of parallelogram faces.

We find the condition that results in situation 1). The BZ face centered on $(-\mathbf{a}'^* + \mathbf{b}'^* + \mathbf{c}'^*)/2$ shares an edge with BZ faces centered on $\mathbf{b}'^*/2$, $\mathbf{c}'^*/2$, $(-\mathbf{a}'^* + \mathbf{b}'^*)/2$ and $(-\mathbf{a}'^* + \mathbf{c}'^*)/2$. The origin, together with $-\mathbf{a}'^* + \mathbf{b}'^* + \mathbf{c}'^*$, must be the two closest lattice points to $(-\mathbf{a}'^* + \mathbf{b}'^* + \mathbf{c}'^*)/2$ for $(-\mathbf{a}'^* + \mathbf{b}'^* + \mathbf{c}'^*)/2$ to be a BZ face center. In other words, the distance from $(-\mathbf{a}'^* + \mathbf{b}'^* + \mathbf{c}'^*)/2$ to $\mathbf{b}'^*$ and $\mathbf{c}'^*$ must be longer than that to the origin. This holds when $\left|-\mathbf{a}'^* + \mathbf{b}'^* + \mathbf{c}'^*\right|^2$ is smaller than both $\left|\mathbf{a}'^* - \mathbf{b}'^* + \mathbf{c}'^*\right|^2$ and $\left|\mathbf{a}'^* + \mathbf{b}'^* - \mathbf{c}'^*\right|^2$, which is equivalent to when $\mathbf{b}'^* \cdot \mathbf{c}'^* = k_b' k_c' \cos k_\alpha'$ is smaller than $\mathbf{c}'^* \cdot \mathbf{a}'^* = k_c' k_a' \cos k_\beta'$ and $\mathbf{a}'^* \cdot \mathbf{b}'^* = k_a' k_b' \cos k_\gamma'$.

The condition that results in situation 2) and 3) can be obtained similarly. Based on this derivation, the "reduced" cell in this study is defined such that $\left|k_{\mathrm{R}a}k_{\mathrm{R}b}\cos k_{\mathrm{R}\gamma}\right|$ is the smallest in the set $\left\{\left|k_{\mathrm{R}b}k_{\mathrm{R}c}\cos k_{\mathrm{R}\alpha}\right|,\left|k_{\mathrm{R}c}k_{\mathrm{R}a}\cos k_{\mathrm{R}\beta}\right|,\left|k_{\mathrm{R}a}k_{\mathrm{R}b}\cos k_{\mathrm{R}\gamma}\right|\right\}$, which guarantees that $\mathbf{c}_{\mathrm{R}}^{*}$ always penetrates a parallelogram face when reciprocal interaxial angles are all-acute.

Appendix D. Space group number ranges relevant in implementation.

Designation of an "extended Bravais symbol" could be useful in implementing code to determine the relevant table of distinctive BZ point labels and coordinates (Tables 69-92) and the appropriate band path. The extended Bravais symbols of four characters; the first two is the Bravais symbol, the third character is the "type" and is either 1, 2, or 3, and the fourth character specifies the inversion symmetry and is either Y or N. Therefore, examples of possible extended Bravais symbols are cP1Y and mC1N (italics are not used).

The first characters can be obtained from the space group number (Table 93) and the second character from the first letter of the Hermann-Mauguin symbol of the standard setting (the first setting that appears in Table A1.4.2.7 of ITB[16]). The matrix $\boldsymbol{P}$ used to convert the crystallographic conventional cell to the crystallographic primitive cell (Table 3) is defined based on the Bravais symbol, which is also the first two letters of the extended Bravais symbol. The third letter is obtained by looking at the space group range or logic based on lattice parameters. Information on the definition of the third characters of the extended Bravais symbol as well as on what table among Tables 69-92 should be used is given in Table 94. Whether the cell has intrinsic inversion symmetry or not can be found by looking at the point group or the space group number. Point groups with inversion and the respective space group number range are shown in Table 95.

One can force the fourth letter of the extended Bravais symbol to be Y if time-inversion symmetry is imposed. Subsequently, the path is doubled, or in other words, the additional wedge must be sampled, if the fourth letter is ultimately N.

Table 1. Definition of basis vectors, lattice parameters, and coordinate triplets (direct space) or $\mathbf{k}$ -vector coefficients (reciprocal space) of various cells used in this study.

Cell type	Basis vectors	Basis vector lengths	Interaxial angles	Coordinate triplets / $\mathbf{k}$ -vector coefficients
Crystallographic conventional	$(\mathbf{a},\mathbf{b},\mathbf{c})$	(a,b,c)	(α,β,γ)	$(x,y,z)^{\mathrm{T}}$
Crystallographic primitive	$(\mathbf{a}_{\mathrm{P}},\mathbf{b}_{\mathrm{P}},\mathbf{c}_{\mathrm{P}})$	$(a_{\mathrm{P}},b_{\mathrm{P}},c_{\mathrm{P}})$	$(\alpha_{\mathrm{P}},\beta_{\mathrm{P}},\gamma_{\mathrm{P}})$	$(x_{\mathrm{P}},y_{\mathrm{P}},z_{\mathrm{P}})^{\mathrm{T}}$
“Reduced”	$(\mathbf{a}_{\mathrm{R}},\mathbf{b}_{\mathrm{R}},\mathbf{c}_{\mathrm{R}})$	$(a_{\mathrm{R}},b_{\mathrm{R}},c_{\mathrm{R}})$	$(\alpha_{\mathrm{R}},\beta_{\mathrm{R}},\gamma_{\mathrm{R}})$	$(x_{\mathrm{R}},y_{\mathrm{R}},z_{\mathrm{R}})^{\mathrm{T}}$
SC standard conventional	$(\mathbf{a}',\mathbf{b}',\mathbf{c}')$	(a',b',c')	(α',β',γ')	$(x',y',z')^{\mathrm{T}}$
SC standard primitive	$(\mathbf{a}'_{\mathrm{P}},\mathbf{b}'_{\mathrm{P}},\mathbf{c}'_{\mathrm{P}})$	$(a'_{\mathrm{P}},b'_{\mathrm{P}},c'_{\mathrm{P}})$	$(\alpha'_{\mathrm{P}},\beta'_{\mathrm{P}},\gamma'_{\mathrm{P}})$	$(x'_{\mathrm{P}},y'_{\mathrm{P}},z'_{\mathrm{P}})^{\mathrm{T}}$
Reciprocal crystallographic conventional	$(\mathbf{a}^*/\mathbf{b}^*/\mathbf{c}^*)$	(k_a,k_b,k_c)	$(k_\alpha,k_\beta,k_\gamma)$	(k_x,k_y,k_z)
Reciprocal crystallographic primitive	$(\mathbf{a}^*_{\mathrm{P}}/\mathbf{b}^*_{\mathrm{P}}/\mathbf{c}^*_{\mathrm{P}})$	$(k_{\mathrm{P}a},k_{\mathrm{P}b},k_{\mathrm{P}c})$	$(k_{\mathrm{P}\alpha},k_{\mathrm{P}\beta},k_{\mathrm{P}\gamma})$	$(k_{\mathrm{P}x},k_{\mathrm{P}y},k_{\mathrm{P}z})$
Reciprocal “ITA description”	$(\mathbf{a}^*_{\mathrm{ITA}}/\mathbf{b}^*_{\mathrm{ITA}}/\mathbf{c}^*_{\mathrm{ITA}})$	$(k_{\mathrm{ITA}a},k_{\mathrm{ITA}b},k_{\mathrm{ITA}c})$	$(k_{\mathrm{ITA}\alpha},k_{\mathrm{ITA}\beta},k_{\mathrm{ITA}\gamma})$	$(k_{\mathrm{ITA}x},k_{\mathrm{ITA}y},k_{\mathrm{ITA}z})$
Reciprocal “reduced”	$(\mathbf{a}^*_{\mathrm{R}}/\mathbf{b}^*_{\mathrm{R}}/\mathbf{c}^*_{\mathrm{R}})$	$(k_{\mathrm{R}a},k_{\mathrm{R}b},k_{\mathrm{R}c})$	$(k_{\mathrm{R}\alpha},k_{\mathrm{R}\beta},k_{\mathrm{R}\gamma})$	$(k_{\mathrm{R}x},k_{\mathrm{R}y},k_{\mathrm{R}z})$
Reciprocal SC standard conventional	$(\mathbf{a}'^*/\mathbf{b}'^*/\mathbf{c}'^*)$	(k'_a,k'_b,k'_c)	$(k'_\alpha,k'_\beta,k'_\gamma)$	(k'_x,k'_y,k'_z)
Reciprocal SC standard primitive	$(\mathbf{a}'^*_{\mathrm{P}}/\mathbf{b}'^*_{\mathrm{P}}/\mathbf{c}'^*_{\mathrm{P}})$	$(k'_{\mathrm{P}a},k'_{\mathrm{P}b},k'_{\mathrm{P}c})$	$(k'_{\mathrm{P}\alpha},k'_{\mathrm{P}\beta},k'_{\mathrm{P}\gamma})$	$(k'_{\mathrm{P}x},k'_{\mathrm{P}y},k'_{\mathrm{P}z})$

Table 2. Definition of $\boldsymbol{P}'$ based on SC [3].

Bravais lattice / condition	$\boldsymbol{P}'$	$\boldsymbol{P}'^{-1}$
cP, *tP*, *hP*, *oP*, *mP*, *hR*	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
cI, *tI*, *oI*	$\frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$
cF, *oF*	$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$
oC, *oA*	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
mC	$\frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 3. Definition of $\boldsymbol{P}$ based on Table 2 of Ref. [10]. *: $\boldsymbol{P}$ for *oA* and *mC* cannot be obtained directly from Table 2 of Ref. [10] (see Appendix B).

Bravais lattice	$\boldsymbol{P}$	$\boldsymbol{P}^{-1}$
cP, *tP*, *hP*, *oP*, *mP*	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
cF, *oF*	$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$
cI, *tI*, *oI*	$\frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$
hR	$\frac{1}{3}\begin{pmatrix} 2 & \bar{1} & \bar{1} \\ 1 & 1 & \bar{2} \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$
oC	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
*oA**	$\frac{1}{2}\begin{pmatrix} 0 & 0 & 2 \\ 1 & 1 & 0 \\ \bar{1} & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & \bar{1} \\ 0 & 1 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
*mC**	$\frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 4. Definition of $\boldsymbol{S}$ based on Hinuma *et al.*[8]

Bravais lattice / condition	$\boldsymbol{S}$	$\boldsymbol{S}^{-1}$
cP, cF, cI, tP, tI, hP	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
hR	$\frac{1}{3}\begin{pmatrix}2&\bar{1}&\bar{1}\\1&1&\bar{2}\\1&1&1\end{pmatrix}$	$\begin{pmatrix}1&0&1\\\bar{1}&1&1\\0&\bar{1}&1\end{pmatrix}$
oP $a<b<c$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oF $a<b<c$ $a^{-2}>b^{-2}+c^{-2}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oF $c<a<b$ $c^{-2}>a^{-2}+b^{-2}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$
oF $a<b<c$ a^{-2},b^{-2},c^{-2} =edges of triangle	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oI $a<b<c$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oI $b<c<a$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$

oI $c < a < b$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
oC $a<b$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
oC $b<a$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
oA $b<c$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
oA $c<b$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$
mP $a<c$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
mC	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 5. Definition of $\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'$ based on Refs. [3, 8, 10]

Centering / condition	$\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'$	$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1}$
cP, cI, cF, tP, tI, hP, hR	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oP $a<b<c$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oF $a<b<c$ $a^{-2}>b^{-2}+c^{-2}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oF $c<a<b$ $c^{-2}>a^{-2}+b^{-2}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$
oF $a<b<c$ a^{-2},b^{-2},c^{-2} =edges of triangle	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oI $a<b<c$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
oI $b<c<a$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$

oI $c<a<b$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
oC $a<b$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
oC $b<a$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
oA $b<c$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
oA $c<b$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
mP $a<c$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
mC	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 6. Definition of $\boldsymbol{Q}$ based on Tables 2 and 3 of Ref. [10] and Table 1.5.4.2 of the ITB [16]. *: $\boldsymbol{Q}$ for *mC* cannot be obtained directly from Tables 2 and 3 of Ref. [10] (see Appendix B).

Bravais lattice	$\boldsymbol{Q}$	$\boldsymbol{Q}^{-1}$
cP, *tP*, *oP*, *mP*	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
cF, *oF*	$\frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$
oI, *cI*	$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$
tI	$\frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 2 & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$
hP	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
hR	$\frac{1}{3}\begin{pmatrix} 2 & 1 & 1 \\ \bar{1} & 1 & 1 \\ \bar{1} & \bar{2} & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}$
oC, *oA*	$\frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

*mC**	$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 7. List of relevant tables and figures by Bravais lattice.

Lattice system	Centering	Symbol	Condition	Tables	Figures
Cubic	Primitive	*cP*		8, 31, 32, 69	2
	Face	*cF*		9, 33, 34, 70	3
	Body	*cI*		10, 35, 36, 71	4
Tetragonal	Primitive	*tP*		11, 37, 38, 72	5
	Body	*tI*	$c < a$	12, 39, 40, 73	6
			$c > a$	13, 41, 42, 74	7
Orthorhombic	Primitive	*oP*		14, 43, 75	8
	Face	*oF*	$a^{-2} > b^{-2} + c^{-2}$	15, 44, 76	9
			$c^{-2} > a^{-2} + b^{-2}$	16, 45, 77	10
			Other	17, 46, 78	11
	Body	*oI*	c largest	18, 47, 79	12
			a largest	19, 48, 80	13
			b largest	20, 49, 81	14
	Side-face	*oS* (*oA*, *oC*)	*1	21, 50, 82	15
			*2	22, 51, 83	16
Hexagonal	Primitive	*hP*		23, 52-56, 84	17
Rhombohedral	Triple	*hR*	$\sqrt{3}a < \sqrt{2}c$	24, 57, 58, 85	18
	hexagonal		$\sqrt{3}a > \sqrt{2}c$	25, 59, 60, 86	19
Monoclinic	Primitive	*mP*		26, 61, 87	20
	Side-face	*mS* (*mC*)	$b < a \sin\beta$	27, 62, 88	21
			*3	28, 63, 89	22
			*4	29, 64, 90	23
Triclinic	Primitive	*aP*	*5	65, 66, 67, 91	24
			*6	65, 66, 68, 92	25

*1: $a < b$ if *oC* or $b < c$ if *oA*

*2: $a > b$ if *oC* or $b > c$ if *oA*

*3: $b > a \sin\beta$ and $-\dfrac{a\cos\beta}{c} + \dfrac{a^2\sin^2\beta}{b^2} < 1$

*4: $b > a \sin\beta$ and $-\dfrac{a\cos\beta}{c} + \dfrac{a^2\sin^2\beta}{b^2} > 1$

*5 Interaxial angles of the reciprocal “reduced” cell are all-obtuse

*6 Interaxial angles of the reciprocal “reduced” cell are all-acute

Table 8. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *cP*.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
M	1/2	1/2	0	1/2	1/2	0	1/2	1/2	0
R	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
X	0	1/2	0	0	1/2	0	0	1/2	0

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\ \ \boldsymbol{Q}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}.$$

Table 9. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *cF*.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
K	3/8	3/8	3/4	3/8	3/8	3/4	3/8	3/8	0
L	1/2	1/2	1/2	1/2	1/2	1/2	1/4	1/4	1/4
U	5/8	1/4	5/8	5/8	1/4	5/8	1/8	1/2	1/8
W	1/2	1/4	3/4	1/2	1/4	3/4	1/4	1/2	0
X	1/2	0	1/2	1/2	0	1/2	0	1/2	0

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\ \ \boldsymbol{Q}=\frac{1}{2}\begin{pmatrix}\bar{1}&1&1\\1&\bar{1}&1\\1&1&\bar{1}\end{pmatrix}.$$

Table 10. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *cI*.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
H	1/2	-1/2	1/2	1/2	-1/2	1/2	0	1/2	0
P	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
N	0	0	1/2	0	0	1/2	1/4	1/4	0

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad \boldsymbol{Q}=\frac{1}{2}\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}.$$

Table 11. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *tP*.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
A	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
M	1/2	1/2	0	1/2	1/2	0	1/2	1/2	0
R	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
X	0	1/2	0	0	1/2	0	0	1/2	0
Z	0	0	1/2	0	0	1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{Q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Table 12. $\mathbf{k}$-vector coefficients of points in reciprocal space defined in Ref. [3] for *tI* when $c' < a'$ $(c < a)$.

Label	$\mathbf{k}$-vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
M	-1/2	1/2	1/2	-1/2	1/2	1/2	1/2	1/2	0
N	0	1/2	0	0	1/2	0	1/4	1/4	1/4
P	1/4	1/4	1/4	1/4	1/4	1/4	0	1/2	1/4
X	0	0	1/2	0	0	1/2	0	1/2	0
Z	η	η	$-\eta$	η	η	$-\eta$	0	0	η
Z_1	$-\eta$	$1-\eta$	η	$-\eta$	$1-\eta$	η	1/2	1/2	$1/2-\eta$

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 2 & 0 \end{pmatrix}, \ \eta = \frac{1}{4}\left(1+\frac{c'^2}{a'^2}\right) = \frac{1}{4}\left(1+\frac{c^2}{a^2}\right).$$

Table 13. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *tI* when $c' > a'$ $(c > a)$.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
N	0	1/2	0	0	1/2	0	1/4	1/4	1/4
P	1/4	1/4	1/4	1/4	1/4	1/4	0	1/2	1/4
Σ	-η	η	η	-η	η	η	η	η	0
Σ_1	η	1-η	-η	η	1-η	-η	1/2-η	1/2-η	1/2
X	0	0	1/2	0	0	1/2	0	1/2	0
Y	-ζ	ζ	1/2	-ζ	ζ	1/2	ζ	1/2	0
Y_1	1/2	1/2	-ζ	1/2	1/2	-ζ	0	1/2-ζ	1/2
Z	1/2	1/2	-1/2	1/2	1/2	-1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 2 & 0 \end{pmatrix} \quad , \quad \eta = \frac{1}{4}\left(1 + \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{a^2}{c^2}\right) \quad ,$$

$$\zeta = \frac{a'^2}{2c'^2} = \frac{a^2}{2c^2} .$$

Table 14. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *oP* when $a < b < c$ $\left(a = a', b = b', c = c'\right)$.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
R	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
S	1/2	1/2	0	1/2	1/2	0	1/2	1/2	0
T	0	1/2	1/2	0	1/2	1/2	0	1/2	1/2
U	1/2	0	1/2	1/2	0	1/2	1/2	0	1/2
X	1/2	0	0	1/2	0	0	1/2	0	0
Y	0	1/2	0	0	1/2	0	0	1/2	0
Z	0	0	1/2	0	0	1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{Q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Table 15. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for *oF* when $a'^{-2} > b'^{-2} + c'^{-2}$ and $a < b < c$ $(a = a', b = b', c = c')$.

Label	$\mathbf{k}$ -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
A	1/2	1/2+ζ	ζ	1/2	1/2+ζ	ζ	ζ	0	1/2
A_1	1/2	1/2-ζ	1-ζ	1/2	1/2-ζ	1-ζ	1/2-ζ	1/2	0
L	1/2	1/2	1/2	1/2	1/2	1/2	1/4	1/4	1/4
T	1	1/2	1/2	1	1/2	1/2	0	1/2	1/2
X	0	η	η	0	η	η	η	0	0
X_1	1	1-η	1-η	1	1-η	1-η	1/2-η	1/2	1/2
Y	1/2	0	1/2	1/2	0	1/2	0	1/2	0
Z	1/2	1/2	0	1/2	1/2	0	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1 + \frac{a'^2}{b'^2} - \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{a^2}{b^2} - \frac{a^2}{c^2}\right),$$

$$\eta = \frac{1}{4}\left(1 + \frac{a'^2}{b'^2} + \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{a^2}{b^2} + \frac{a^2}{c^2}\right).$$

Table 16. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *oF* when $a'^{-2} > b'^{-2} + c'^{-2}$ and $c < a < b$ $\left(c = a', a = b', b = c'\right)$.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	k'_{Pz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
A	1/2	1/2+ζ	ζ	1/2+ζ	ζ	1/2	0	1/2	ζ
A_1	1/2	1/2-ζ	1-ζ	1/2-ζ	1-ζ	1/2	1/2	0	1/2-ζ
L	1/2	1/2	1/2	1/2	1/2	1/2	1/4	1/4	1/4
T	1	1/2	1/2	1/2	1/2	1	1/2	1/2	0
X	0	η	η	η	η	0	0	0	η
X_1	1	1-η	1-η	1-η	1-η	1	1/2	1/2	1/2-η
Y	1/2	0	1/2	0	1/2	1/2	1/2	0	0
Z	1/2	1/2	0	1/2	0	1/2	0	1/2	0

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1 + \frac{a'^2}{b'^2} - \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{c^2}{a^2} - \frac{c^2}{b^2}\right),$$

$$\eta = \frac{1}{4}\left(1 + \frac{a'^2}{b'^2} + \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{c^2}{a^2} + \frac{c^2}{b^2}\right).$$

Table 17. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for *oF* when $a'^{-2} < b'^{-2} + c'^{-2}$ and $a < b < c$ $\left(a = a', b = b', c = c'\right)$.

Label	$\mathbf{k}$ -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
C	1/2	1/2-η	1-η	1/2	1/2-η	1-η	1/2-η	1/2	0
C_1	1/2	1/2+η	η	1/2	1/2+η	η	η	0	1/2
D	1/2-δ	1/2	1-δ	1/2-δ	1/2	1-δ	1/2	1/2-δ	0
D_1	1/2+δ	1/2	δ	1/2+δ	1/2	δ	0	δ	1/2
L	1/2	1/2	1/2	1/2	1/2	1/2	1/4	1/4	1/4
H	1-ϕ	1/2-ϕ	1/2	1-ϕ	1/2-ϕ	1/2	0	1/2	1/2-ϕ
H_1	ϕ	1/2+ ϕ	1/2	ϕ	1/2+ ϕ	1/2	1/2	0	ϕ
X	0	1/2	1/2	0	1/2	1/2	1/2	0	0
Y	1/2	0	1/2	1/2	0	1/2	0	1/2	0
Z	1/2	1/2	0	1/2	1/2	0	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}, \quad \eta = \frac{1}{4}\left(1 + \frac{a'^2}{b'^2} - \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{a^2}{b^2} - \frac{a^2}{c^2}\right),$$

$$\delta = \frac{1}{4}\left(1 + \frac{b'^2}{a'^2} - \frac{b'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{b^2}{a^2} - \frac{b^2}{c^2}\right), \quad \phi = \frac{1}{4}\left(1 + \frac{c'^2}{b'^2} - \frac{c'^2}{a'^2}\right) = \frac{1}{4}\left(1 + \frac{c^2}{b^2} - \frac{c^2}{a^2}\right).$$

Table 18. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for *oI* when $a < b < c$ $\left(a = a', b = b', c = c'\right)$.

Label	$\mathbf{k}$ -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	k'_{Pz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
L	$-\mu$	μ	$1/2-\delta$	$-\mu$	μ	$1/2-\delta$	ζ	$1/2-\eta$	0
L_1	μ	$-\mu$	$1/2+\delta$	μ	$-\mu$	$1/2+\delta$	$1/2-\zeta$	η	0
L_2	$1/2-\delta$	$1/2+\delta$	$-\mu$	$1/2-\delta$	$1/2+\delta$	$-\mu$	$1/2-\zeta$	$1/2-\eta$	1/2
R	0	1/2	0	0	1/2	0	1/4	0	1/4
S	1/2	0	0	1/2	0	0	0	1/4	1/4
T	0	0	1/2	0	0	1/2	1/4	1/4	0
W	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
X	$-\zeta$	ζ	ζ	$-\zeta$	ζ	ζ	ζ	0	0
X_1	ζ	$1-\zeta$	$-\zeta$	ζ	$1-\zeta$	$-\zeta$	$1/2-\zeta$	0	1/2
Y	η	$-\eta$	η	η	$-\eta$	η	0	η	0
Y_1	$1-\eta$	η	$-\eta$	$1-\eta$	η	$-\eta$	0	$1/2-\eta$	1/2
Z	1/2	1/2	-1/2	1/2	1/2	-1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad , \quad \zeta = \frac{1}{4}\left(1 + \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{a^2}{c^2}\right) \quad ,$$

$$\eta = \frac{1}{4}\left(1 + \frac{b'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{b^2}{c^2}\right), \quad \delta = \frac{b'^2 - a'^2}{4c'^2} = \frac{b^2 - a^2}{4c^2}, \quad \mu = \frac{a'^2 + b'^2}{4c'^2} = \frac{a^2 + b^2}{4c^2} \,.$$

Table 19. **k**-vector coefficients of points in reciprocal space defined in Ref. [3] for *oI* when $b < c < a$ $(b = a', c = b', a = c')$.

Label	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	k'_{Pz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
	k-vector coefficients								
Γ	0	0	0	0	0	0	0	0	0
L	-μ	μ	1/2-δ	1/2-δ	-μ	μ	0	ζ	1/2-η
L_1	μ	-μ	1/2+δ	1/2+δ	μ	-μ	0	1/2-ζ	η
L_2	1/2-δ	1/2+δ	-μ	-μ	1/2-δ	1/2+δ	1/2	1/2-ζ	1/2-η
R	0	1/2	0	0	0	1/2	1/4	1/4	0
S	1/2	0	0	0	1/2	0	1/4	0	1/4
T	0	0	1/2	1/2	0	0	0	1/4	1/4
W	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
X	-ζ	ζ	ζ	ζ	-ζ	ζ	0	ζ	0
X_1	ζ	1-ζ	-ζ	-ζ	ζ	1-ζ	1/2	1/2-ζ	0
Y	η	-η	η	η	η	-η	0	0	η
Y_1	1-η	η	-η	-η	1-η	η	1/2	0	1/2-η
Z	1/2	1/2	-1/2	-1/2	1/2	1/2	1/2	0	0

$$(\boldsymbol{P}^{-1}\boldsymbol{SP}')^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad , \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad , \quad \zeta = \frac{1}{4}\left(1 + \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{b^2}{a^2}\right) \quad ,$$

$$\eta = \frac{1}{4}\left(1 + \frac{b'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{c^2}{a^2}\right), \;\; \delta = \frac{b'^2 - a'^2}{4c'^2} = \frac{c^2 - b^2}{4a^2}, \;\; \mu = \frac{a'^2 + b'^2}{4c'^2} = \frac{b^2 + c^2}{4a^2}.$$

Table 20. $\mathbf{k}$-vector coefficients of points in reciprocal space defined in Ref. [3] for *oI* when $c < a < b \quad (c = a', a = b', b = c')$.

Label	$\mathbf{k}$-vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	k'_{Pz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
L	$-\mu$	μ	$1/2-\delta$	μ	$1/2-\delta$	$-\mu$	$1/2-\eta$	0	ζ
L_1	μ	$-\mu$	$1/2+\delta$	$-\mu$	$1/2+\delta$	μ	η	0	$1/2-\zeta$
L_2	$1/2-\delta$	$1/2+\delta$	$-\mu$	$1/2+\delta$	$-\mu$	$1/2-\delta$	$1/2-\eta$	1/2	$1/2-\zeta$
R	0	1/2	0	1/2	0	0	0	1/4	1/4
S	1/2	0	0	0	0	1/2	1/4	1/4	0
T	0	0	1/2	0	1/2	0	1/4	0	1/4
W	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
X	$-\zeta$	ζ	ζ	ζ	ζ	$-\zeta$	0	0	ζ
X_1	ζ	$1-\zeta$	$-\zeta$	$1-\zeta$	$-\zeta$	ζ	0	1/2	$1/2-\zeta$
Y	η	$-\eta$	η	$-\eta$	η	η	η	0	0
Y_1	$1-\eta$	η	$-\eta$	η	$-\eta$	$1-\eta$	$1/2-\eta$	1/2	0
Z	1/2	1/2	-1/2	1/2	-1/2	1/2	0	1/2	0

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad , \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad , \quad \zeta = \frac{1}{4}\left(1 + \frac{a'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{c^2}{b^2}\right) \quad ,$$

$$\eta = \frac{1}{4}\left(1 + \frac{b'^2}{c'^2}\right) = \frac{1}{4}\left(1 + \frac{a^2}{b^2}\right), \quad \delta = \frac{b'^2 - a'^2}{4c'^2} = \frac{a^2 - c^2}{4b^2}, \quad \mu = \frac{a'^2 + b'^2}{4c'^2} = \frac{c^2 + a^2}{4b^2}.$$

Table 21. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *oC* when $a < b$ $\left(a = a', b = b', c = c'\right)$ and *oA* where $b < c$ $\left(b = a', c = b', a = c'\right)$

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
A	ζ	ζ	1/2	ζ	ζ	1/2	ζ	0	1/2
A_1	-ζ	1-ζ	1/2	-ζ	1-ζ	1/2	1/2-ζ	1/2	1/2
R	0	1/2	1/2	0	1/2	1/2	1/4	1/4	1/2
S	0	1/2	0	0	1/2	0	1/4	1/4	0
T	-1/2	1/2	1/2	-1/2	1/2	1/2	0	1/2	1/2
X	ζ	ζ	0	ζ	ζ	0	ζ	0	0
X_1	-ζ	1-ζ	0	-ζ	1-ζ	0	1/2-ζ	1/2	0
Y	-1/2	1/2	0	-1/2	1/2	0	0	1/2	0
Z	0	0	1/2	0	0	1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1 + \frac{a'^2}{b'^2}\right).$$

Table 22. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for *oC* when $b < a \quad (b = a', a = b', c = c')$ and *oA* where $c < b \quad (c = a', b = b', a = c')$

Label	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
	k -vector coefficients								
Γ	0	0	0	0	0	0	0	0	0
A	ζ	ζ	1/2	$-\zeta$	ζ	-1/2	0	ζ	-1/2
A_1	$-\zeta$	$1-\zeta$	1/2	ζ	$1-\zeta$	-1/2	1/2	$1/2-\zeta$	-1/2
R	0	1/2	1/2	0	1/2	-1/2	1/4	1/4	-1/2
S	0	1/2	0	0	1/2	0	1/4	1/4	0
T	-1/2	1/2	1/2	1/2	1/2	-1/2	1/2	0	-1/2
X	ζ	ζ	0	$-\zeta$	ζ	0	0	ζ	0
X_1	$-\zeta$	$1-\zeta$	0	ζ	$1-\zeta$	0	1/2	$1/2-\zeta$	0
Y	-1/2	1/2	0	1/2	1/2	0	1/2	0	0
Z	0	0	1/2	0	0	-1/2	0	0	-1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1 + \frac{a'^2}{b'^2}\right).$$

Table 23. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *hP*.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
A	0	0	1/2	0	0	1/2	0	0	1/2
H	1/3	1/3	1/2	1/3	1/3	1/2	2/3	1/3	1/2
K	1/3	1/3	0	1/3	1/3	0	2/3	1/3	0
L	1/2	0	1/2	1/2	0	1/2	1/2	0	1/2
M	1/2	0	0	1/2	0	0	1/2	0	0

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad \boldsymbol{Q}=\begin{pmatrix}1&0&0\\1&1&0\\0&0&1\end{pmatrix}.$$

Table 24. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *hR* when $\sqrt{3}a < \sqrt{2}c \quad (\alpha' < 90^\circ)$.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	k'_{Pz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	k_{ITAz}
Γ	0	0	0	0	0	0	0	0	0
B	η	1/2	1-η	η	1/2	1-η	1/3-2δ	1/3-2δ	1/2
B_1	1/2	1-η	η-1	1/2	1-η	-1+η	1/3	1/3+2δ	1/6
F	1/2	1/2	0	1/2	1/2	0	1/6	1/3	1/3
L	1/2	0	0	1/2	0	0	1/3	1/6	1/6
L_1	0	0	-1/2	0	0	-1/2	1/6	1/3	-1/6
P	η	ν	ν	η	ν	ν	1/3-2δ	1/6-δ	1/2
P_1	1-ν	1-ν	1-η	1-ν	1-ν	1-η	1/6-δ	1/3-2δ	1/2
P_2	ν	ν	η-1	ν	ν	-1+η	1/6+δ	1/3+2δ	1/6
Q	1-ν	ν	0	1-ν	ν	0	1/3-δ	1/3	1/3
X	ν	0	-ν	ν	0	-ν	1/3+δ	1/3+δ	0
Z	1/2	1/2	1/2	1/2	1/2	1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad \boldsymbol{Q} = \frac{1}{3}\begin{pmatrix} 2 & 1 & 1 \\ \bar{1} & 1 & 1 \\ \bar{1} & \bar{2} & 1 \end{pmatrix} \quad , \quad \eta = \frac{1+4\cos\alpha'}{2+4\cos\alpha'} = \frac{5}{6} - \frac{a^2}{2c^2} \quad ,$$

$$\nu = \frac{3}{4} - \frac{\eta}{2} = \frac{1}{3} + \frac{a^2}{4c^2}, \quad \delta = \frac{a^2}{4c^2}, \quad a' = \frac{\sqrt{3a^2 + c^2}}{3}, \quad \cos\alpha' = \frac{-3a^2 + 2c^2}{6a^2 + 2c^2}.$$

Table 25. **k** -vector coefficients of points in reciprocal space defined in Ref. [3] for *hR* when $\sqrt{3}a > \sqrt{2}c \quad (\alpha' > 90^\circ)$.

Label	**k** -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	k'_{Pz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
F	1/2	-1/2	0	1/2	-1/2	0	1/2	0	0
L	1/2	0	0	1/2	0	0	1/3	1/6	1/6
P	1-ν	-ν	1-ν	1-ν	-ν	1-ν	1/3	-1/3	1/6-ζ
P_1	ν	ν-1	ν-1	ν	ν-1	ν-1	2/3	1/3	-1/6+ζ
Q	η	η	η	η	η	η	0	0	1/2-2ζ
Q_1	1-η	-η	-η	1-η	-η	-η	2/3	1/3	-1/6+2ζ
Z	1/2	-1/2	1/2	1/2	-1/2	1/2	1/3	-1/3	1/6

$$\left(\boldsymbol{P}^{-1}\boldsymbol{SP}'\right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad \boldsymbol{Q} = \frac{1}{3}\begin{pmatrix} 2 & 1 & 1 \\ \bar{1} & 1 & 1 \\ \bar{1} & \bar{2} & 1 \end{pmatrix} \quad , \quad \eta = \frac{1}{2\tan^2(\alpha'/2)} = \frac{1}{6} + \frac{2c^2}{9a^2} \quad ,$$

$$\nu = \frac{3}{4} - \frac{\eta}{2} = \frac{2}{3} - \frac{c^2}{9a^2}, \quad \zeta = \nu - \frac{1}{2} = \frac{1}{6} - \frac{c^2}{9a^2}, \quad a' = \frac{\sqrt{3a^2 + c^2}}{3}, \quad \cos\alpha' = \frac{-3a^2 + 2c^2}{6a^2 + 2c^2}.$$

Table 26. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for *mP* when $a < c$ $\left(b = a', a = b', c = c', -\cos\beta = \cos\alpha'\right)$.

Label	$\mathbf{k}$ -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
A	1/2	1/2	0	-1/2	1/2	0	-1/2	1/2	0
C	0	1/2	1/2	-1/2	0	1/2	-1/2	0	1/2
D	1/2	0	1/2	0	1/2	1/2	0	1/2	1/2
D_1	1/2	0	-1/2	0	1/2	-1/2	0	1/2	-1/2
E	1/2	1/2	1/2	-1/2	1/2	1/2	-1/2	1/2	1/2
H	0	η	1-ν	-η	0	1-ν	-η	0	1-ν
H_1	0	1-η	ν	-1+η	0	ν	-1+η	0	ν
H_2	0	η	-ν	-η	0	-ν	-η	0	-ν
M	1/2	η	1-ν	-η	1/2	1-ν	-η	1/2	1-ν
M_1	1/2	1-η	ν	-1+η	1/2	ν	-1+η	1/2	ν
M_2	1/2	η	-ν	-η	1/2	-ν	-η	1/2	-ν
X	0	1/2	0	-1/2	0	0	-1/2	0	0
Y	0	0	1/2	0	0	1/2	0	0	1/2
Y_1	0	0	-1/2	0	0	-1/2	0	0	-1/2
Z	1/2	0	0	0	1/2	0	0	1/2	0

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad \boldsymbol{Q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \quad \eta = \frac{1-\left(b'/c'\right)\cos\alpha'}{2\sin^2\alpha'} = \frac{1+\left(a/c\right)\cos\beta}{2\sin^2\beta} \quad ,$$

$$\nu = \frac{1}{2} - \frac{\eta c'\cos\alpha'}{b'} = \frac{1}{2} + \frac{\eta c\cos\beta}{a} .$$

Table 27. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for *mC* when $b < a\sin\beta$ $\left(k'_{\mathrm{P}\gamma} > 90^\circ\right)$ $\left(b = a', a = b', c = c', -\cos\beta = \cos\alpha'\right)$.

Label	$\mathbf{k}$ -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
N	1/2	0	0	0	1/2	0	-1/4	1/4	0
N_1	0	-1/2	0	1/2	0	0	1/4	1/4	0
F	1-ζ	1-ζ	1-η	-1+ζ	1-ζ	1-η	-1+ζ	0	1-η
F_1	ζ	ζ	η	-ζ	ζ	η	-ζ	0	η
F_2	-ζ	-ζ	1-η	ζ	-ζ	1-η	ζ	0	1-η
I	ϕ	1-ϕ	1/2	-1+ϕ	ϕ	1/2	-1/2	-1/2+ϕ	1/2
I_1	1-ϕ	ϕ-1	1/2	1-ϕ	1- ϕ	1/2	0	1-ϕ	1/2
L	1/2	1/2	1/2	-1/2	1/2	1/2	-1/2	0	1/2
M	1/2	0	1/2	0	1/2	1/2	-1/4	1/4	1/2
X	1-ψ	ψ-1	0	1-ψ	1-ψ	0	0	1-ψ	0
X_1	ψ	1-ψ	0	-1+ψ	ψ	0	-1/2	-1/2+ψ	0
X_2	ψ-1	-ψ	0	ψ	-1+ψ	0	1/2	-1/2+ψ	0
Y	1/2	1/2	0	-1/2	1/2	0	-1/2	0	0
Y_1	-1/2	-1/2	0	1/2	-1/2	0	1/2	0	0
Z	0	0	1/2	0	0	1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \zeta = \frac{2-\left(b'/c'\right)\cos\alpha'}{4\sin^2\alpha'} = \frac{2+\left(a/c\right)\cos\beta}{4\sin^2\beta},$$

$$\eta = \frac{1}{2} + \frac{2\zeta c'\cos\alpha'}{b'} = \frac{1}{2} - \frac{2\zeta c\cos\beta}{a}, \qquad \psi = \frac{3}{4} - \frac{a'^2}{4b'^2\sin^2\alpha'} = \frac{3}{4} - \frac{b^2}{4a^2\sin^2\beta},$$

$$\phi = \psi + \left(\frac{3}{4} - \psi\right)\frac{b'\cos\alpha'}{c'} = \psi - \left(\frac{3}{4} - \psi\right)\frac{a\cos\beta}{c}.$$

Table 28. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for mC when $b > a\sin\beta$ and $-\dfrac{a\cos\beta}{c}+\dfrac{a^2\sin^2\beta}{b^2}<1$ ($k'_{\mathrm{P}\gamma}<90^\circ$ and $\dfrac{b'\cos\alpha'}{c'}+\dfrac{b'^2\sin^2\alpha'}{a'^2}<1$) $\left(b=a', a=b', c=c', -\cos\beta=\cos\alpha'\right)$.

Label	$\mathbf{k}$ -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
F	1-ϕ	1-ϕ	1-ψ	-1+ϕ	1-ϕ	1-ψ	-1+ϕ	0	1-ψ
F_1	ϕ	ϕ-1	ψ	1-ϕ	ϕ	ψ	1/2-ϕ	1/2	ψ
F_2	1-ϕ	-ϕ	1-ψ	ϕ	1-ϕ	1-ψ	-1/2+ϕ	1/2	1-ψ
H	ζ	ζ	η	-ζ	ζ	η	-ζ	0	η
H_1	1-ζ	-ζ	1-η	ζ	1-ζ	1-η	-1/2+ζ	1/2	1-η
H_2	-ζ	-ζ	1-η	ζ	-ζ	1-η	ζ	0	1-η
I	1/2	-1/2	1/2	1/2	1/2	1/2	0	1/2	1/2
M	1/2	0	1/2	0	1/2	1/2	-1/4	1/4	1/2
N	1/2	0	0	0	1/2	0	-1/4	1/4	0
N_1	0	-1/2	0	1/2	0	0	1/4	1/4	0
X	1/2	-1/2	0	1/2	1/2	0	0	1/2	0
Y	μ	μ	δ	-μ	μ	δ	-μ	0	δ
Y_1	1-μ	-μ	-δ	μ	1-μ	-δ	-1/2+μ	1/2	-δ
Y_2	-μ	-μ	-δ	μ	-μ	-δ	μ	0	-δ
Y_3	μ	μ-1	δ	1-μ	μ	δ	1/2-μ	1/2	δ
Z	0	0	1/2	0	0	1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{SP}'\right)^{-1}=\begin{pmatrix}0&1&0\\\bar{1}&0&0\\0&0&1\end{pmatrix}\quad,\qquad \boldsymbol{Q}=\frac{1}{2}\begin{pmatrix}1&1&0\\\bar{1}&1&0\\0&0&2\end{pmatrix}\quad,\qquad \mu=\frac{1}{4}\left(1+\frac{b'^2}{a'^2}\right)=\frac{1}{4}\left(1+\frac{a^2}{b^2}\right)\quad,$$

$$\delta=\frac{b'c'\cos\alpha'}{2a'^2}=-\frac{ac\cos\beta}{2b^2}\ ,\quad \zeta=\frac{1}{4}\left(\frac{b'^2}{a'^2}+\frac{1-(b'/c')\cos\alpha'}{\sin^2\alpha'}\right)=\frac{1}{4}\left(\frac{a^2}{b^2}+\frac{1+(a/c)\cos\beta}{\sin^2\beta}\right),$$

$$\eta=\frac{1}{2}+\frac{2\zeta c'\cos\alpha'}{b'}=\frac{1}{2}-\frac{2\zeta c\cos\beta}{a},\ \ \phi=1+\zeta-2\mu,\ \ \psi=\eta-2\delta\,.$$

Table 29. $\mathbf{k}$ -vector coefficients of points in reciprocal space defined in Ref. [3] for *mC* when $b > a\sin\beta$ and $-\dfrac{a\cos\beta}{c}+\dfrac{a^2\sin^2\beta}{b^2}>1$ ($k'_{\mathrm{P}\gamma}<90^\circ$ and $\dfrac{b'\cos\alpha'}{c'}+\dfrac{b'^2\sin^2\alpha'}{a'^2}>1$) $(b=a', a=b', c=c', -\cos\beta=\cos\alpha')$.

Label	$\mathbf{k}$ -vector coefficients								
	$k'_{\mathrm{P}x}$	$k'_{\mathrm{P}y}$	$k'_{\mathrm{P}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$
Γ	0	0	0	0	0	0	0	0	0
F	ν	ν	ω	$-\nu$	ν	ω	$-\nu$	0	ω
F_1	$1-\nu$	$1-\nu$	$1-\omega$	$-1+\nu$	$1-\nu$	$1-\omega$	$-1+\nu$	0	$1-\omega$
F_2	ν	$\nu-1$	ω	$1-\nu$	ν	ω	$1/2-\nu$	1/2	ω
H	ζ	ζ	η	$-\zeta$	ζ	η	$-\zeta$	0	η
H_1	$1-\zeta$	$-\zeta$	$1-\eta$	ζ	$1-\zeta$	$1-\eta$	$-1/2+\zeta$	1/2	$1-\eta$
H_2	$-\zeta$	$-\zeta$	$1-\eta$	ζ	$-\zeta$	$1-\eta$	ζ	0	$1-\eta$
I	ρ	$1-\rho$	1/2	$-1+\rho$	ρ	1/2	-1/2	$-1/2+\rho$	1/2
I_1	$1-\rho$	$\rho-1$	1/2	$1-\rho$	$1-\rho$	1/2	0	$1-\rho$	1/2
L	1/2	1/2	1/2	-1/2	1/2	1/2	-1/2	0	1/2
M	1/2	0	1/2	0	1/2	1/2	-1/4	1/4	1/2
N	1/2	0	0	0	1/2	0	-1/4	1/4	0
N_1	0	-1/2	0	1/2	0	0	1/4	1/4	0
X	1/2	-1/2	0	1/2	1/2	0	0	1/2	0
Y	μ	μ	δ	$-\mu$	μ	δ	$-\mu$	0	δ
Y_1	$1-\mu$	$-\mu$	$-\delta$	μ	$1-\mu$	$-\delta$	$-1/2+\mu$	1/2	$-\delta$
Y_2	$-\mu$	$-\mu$	$-\delta$	μ	$-\mu$	$-\delta$	μ	0	$-\delta$
Y_3	μ	$\mu-1$	δ	$1-\mu$	μ	δ	$1/2-\mu$	1/2	δ
Z	0	0	1/2	0	0	1/2	0	0	1/2

$$\left(\boldsymbol{P}^{-1}\boldsymbol{S}\boldsymbol{P}'\right)^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \qquad \boldsymbol{Q} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad ,$$

$$\zeta = \frac{1}{4}\left(\frac{b'^2}{a'^2} + \frac{1-(b'/c')\cos\alpha'}{\sin^2\alpha'}\right) = \frac{1}{4}\left(\frac{a^2}{b^2} + \frac{1+(a/c)\cos\beta}{\sin^2\beta}\right) \quad ,$$

$$\mu = \frac{\eta}{2} + \frac{b'^2}{4a'^2} - \frac{b'c'\cos\alpha'}{2a'^2} = \frac{\eta}{2} + \frac{a^2}{4b^2} + \frac{ac\cos\beta}{2b^2} \quad ,$$

$$\omega = \frac{c'}{2b'\cos\alpha'}\left(-1+4\nu - \frac{b'^2\sin^2\alpha'}{a'^2}\right) = \frac{c}{2a\cos\beta}\left(1-4\nu + \frac{a^2\sin^2\beta}{b^2}\right) \quad ,$$

$$\eta = \frac{1}{2} + \frac{2\zeta c'\cos\alpha'}{b'} = \frac{1}{2} - \frac{2\zeta c\cos\beta}{a} \quad , \quad \delta = -\frac{1}{4} + \frac{\omega}{2} + \frac{\zeta c'\cos\alpha'}{b'} = -\frac{1}{4} + \frac{\omega}{2} - \frac{\zeta c\cos\beta}{a} \quad ,$$

$$\nu = 2\mu - \zeta \, , \quad \rho = 1 - \frac{\zeta a'^2}{b'^2} = 1 - \frac{\zeta b^2}{a^2} \, .$$

Table 30. Corresponding centrosymmetric symmorphic space group type G by space group number and centering.

Crystal system	Number	Centering				
		P	F	I	A, C	R
Triclinic	1-2	$P\bar{1}$				
Monoclinic	3-15	$P2/m$			$C2/m$	
Orthorhombic	16-74	$Pmmm$	$Fmmm$	$Immm$	$Cmmm$	
Tetragonal	75-88	$P4/m$		$I4/m$		
	89-142	$P4/mmm$		$I4/mmm$		
Trigonal	143-148	$P\bar{3}$				$R\bar{3}$
	149-167	*				$R\bar{3}m$
Hexagonal	168-176	$P6/m$				
	177-194	$P6/mmm$				
Cubic	195-206	$Pm\bar{3}$	$Fm\bar{3}$	$Im\bar{3}$		
	207-230	$Pm\bar{3}m$	$Fm\bar{3}m$	$Im\bar{3}m$		

*: $P\bar{3}1m$ if 149, 151, 153, 157, or 159-163, $P\bar{3}m1$ otherwise.

Table 31. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Pm\overline{3}m$. G^* is $(Pm\overline{3}m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1*a*	Γ	Γ	Γ	0	0	0	
1*b*	*R*	*R*	*R*	1/2	1/2	1/2	
3*c*	*M*	*M*	*M*	1/2	1/2	0	
3*d*	*X*	*X*	*X*	0	1/2	0	
6*e*	Δ		Γ-*X*	0	*y*	0	$0 < y < 1/2$
6*f*	*T*		*M*-*R*	1/2	1/2	*z*	$0 < z < 1/2$
6*g*	Λ		Γ-*R*	*x*	*x*	*x*	$0 < x < 1/2$
12*h*	*Z*		*X*-*M*	*x*	1/2	0	$0 < x < 1/2$
12*i*	Σ		Γ-*M*	*x*	*x*	0	$0 < x < 1/2$
12*j*	*S*		*X*-*R*	*x*	1/2	*x*	$0 < x < 1/2$

Table 32. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Pm\bar{3}$. G^* is $(Pm\bar{3})^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1a	Γ	Γ	Γ	0	0	0	
1b	R	R	R	1/2	1/2	1/2	
3c	M	M	M	1/2	1/2	0	
3d	X	X	X	0	1/2	0	
3d	X_1		X_1	1/2	0	0	
6e	Δ		Γ-X	0	y	0	$0 < y < 1/2$
6f	ZA		X_1-M	1/2	y	0	$0 < y < 1/2$
6g	Z		X-M	x	1/2	0	$0 < x < 1/2$
6h	T		M-R	1/2	1/2	z	$0 < z < 1/2$
8i	Λ		Γ-R	x	x	x	$0 < x < 1/2$

Table 33. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Fm\overline{3}m$. G^* is $(Im\overline{3}m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	k_{ITAz}	
2a	Γ	Γ	Γ	0	0	0	
6b	X	X	X	0	1/2	0	
8c	L	L	L	1/4	1/4	1/4	
12d	W	W	W	1/4	1/2	0	
12e	Δ		Γ-X	0	y	0	$0 < y < 1/2$
16f	Λ		Γ-L	x	x	x	$0 < x < 1/4$
24g	V		X-W	x	1/2	0	$0 < x < 1/4$
24h	Σ		Γ-K	x	x	0	$0 < x < 3/8$
24h	S		X-U	x	1/2	x	$0 < x < 1/8$
24h	K	K	K	3/8	3/8	0	
24h	U	U	U	1/8	1/2	1/8	
48i	Q		W-L	1/4	1/2-y	y	$0 < y < 1/4$

24h=(Γ-K)+(U-X).

Table 34. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Fm\bar{3}$. G^* is $(Im\bar{3})^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2*a*	Γ	Γ	Γ	0	0	0	
6*b*	*X*	*X*	*X*	0	1/2	0	
8*c*	*L*	*L*	*L*	1/4	1/4	1/4	
12*d*	Δ		Γ-*X*	0	y	0	$0 < y < 1/2$
12*e*	*V*		*X*-*W*	x	1/2	0	$0 < x < 1/4$
12*e*	*VA*			1/2	y	0	$0 < y < 1/4$
12*e*			X-W_2	0	1/2	z	$0 < z < 1/4$
12*e*	*W*	*W*	*W*	1/4	1/2	0	
12*e*			W_2	0	1/2	1/4	
16*f*	Λ		Γ-*L*	x	x	x	$0 < x < 1/4$
(24*g*)	*K*	*K*	*K*	3/8	3/8	0	
(24*g*)	*U*	*U*	*U*	1/8	1/2	1/8	

12*e*=(X-W)+(W_2-X).

Table 35. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Im\bar{3}m$. G^* is $(Fm\bar{3}m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
4*a*	Γ	Γ	Γ	0	0	0	
4*b*	*H*	*H*	*H*	0	1/2	0	
8*c*	*P*	*P*	*P*	1/4	1/4	1/4	
24*d*	*N*	*N*	*N*	1/4	1/4	0	
24*e*	Δ		Γ-*H*	0	*y*	0	$0 < y < 1/2$
32*f*	Λ		Γ-*P*	*x*	*x*	*x*	$0 < x < 1/4$
32*f*	*F*		*H*-*P*	*x*	1/2-*x*	*x*	$0 < x < 1/4$
48*g*	*D*		*N*-*P*	1/4	1/4	*z*	$0 < z < 1/4$
48*h*	Σ		Γ-*N*	*x*	*x*	0	$0 < x < 1/4$
48*i*	*G*		*H*-*N*	*x*	1/2-*x*	0	$0 < x < 1/4$

32*f*=(Γ-*P*)+(*P*-*H*).

Table 36. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Im\overline{3}$. G^{*} is $(Fm\overline{3})^{*}$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
4*a*	Γ	Γ	Γ	0	0	0	
4*b*	*H*	*H*	*H*	0	1/2	0	
8*c*	*P*	*P*	*P*	1/4	1/4	1/4	
24*d*	*N*	*N*	*N*	1/4	1/4	0	
24*e*	Δ		Γ-*H*	0	*y*	0	$0 < y < 1/2$
32*f*	Λ		Γ-*P*	*x*	*x*	*x*	$0 < x < 1/4$
32*f*	*F*		*H*-*P*	*x*	1/2-*x*	*x*	$0 < x < 1/4$
48*g*	*D*		*N*-*P*	1/4	1/4	*z*	$0 < z < 1/4$

32*f*=(Γ-*P*)+(*P*-*H*).

Table 37. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P4/mmm$. G^* is $(P4/mmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\text{ITA}x}$	$k_{\text{ITA}y}$	$k_{\text{ITA}z}$	
1a	Γ	Γ	Γ	0	0	0	
1b	Z	Z	Z	0	0	1/2	
1c	M	M	M	1/2	1/2	0	
1d	A	A	A	1/2	1/2	1/2	
2e	R	R	R	0	1/2	1/2	
2f	X	X	X	0	1/2	0	
2g	Λ		Γ-Z	0	0	z	$0 < z < 1/2$
2h	V		M-A	1/2	1/2	z	$0 < z < 1/2$
4i	W		X-R	0	1/2	z	$0 < z < 1/2$
4j	Σ		Γ-M	x	x	0	$0 < x < 1/2$
4k	S		Z-A	x	x	1/2	$0 < x < 1/2$
4l	Δ		Γ-X	0	y	0	$0 < y < 1/2$
4m	U		Z-R	0	y	1/2	$0 < y < 1/2$
4n	Y		X-M	x	1/2	0	$0 < x < 1/2$
4o	T		R-A	x	1/2	1/2	$0 < x < 1/2$

Table 38. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P4/m$. G^* is $(P4/m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1a	Γ	Γ	Γ	0	0	0	
1b	Z	Z	Z	0	0	1/2	
1c	M	M	M	1/2	1/2	0	
1d	A	A	A	1/2	1/2	1/2	
2e	X	X	X	0	1/2	0	
2f	R	R	R	0	1/2	1/2	
2g	Λ		Γ-Z	0	0	z	$0 < z < 1/2$
2h	V		M-A	1/2	1/2	z	$0 < z < 1/2$
4i	W		X-R	0	1/2	z	$0 < z < 1/2$

Table 39. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $I4/mmm$ and $c < a$. G^* is $(I4/mmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2*a*	Γ	Γ	Γ	0	0	0	
2*b*	*M*	*M*	*M*	1/2	1/2	0	
4*c*	*X*	*X*	*X*	0	1/2	0	
4*d*	*P*	*P*	*P*	0	1/2	1/4	
4*e*	Λ		Γ-*Z*	0	0	*z*	$0 < z < \eta$
4*e*	*V*		M-Z_0	1/2	1/2	*z*	$0 < z < 1/2 - \eta$
4*e*	*Z*	*Z*	*Z*	0	0	η	
4*e*	Z_0	Z_1	Z_0	1/2	1/2	1/2-η	
8*f*	*N*	*N*	*N*	1/4	1/4	1/4	
8*g*	*W*		*X*-*P*	0	1/2	*z*	$0 < z < 1/4$
8*h*	Σ		Γ-*M*	*x*	*x*	0	$0 < x < 1/2$
8*i*	Δ		Γ-*X*	0	*y*	0	$0 < y < 1/2$
8*j*	*Y*		*X*-*M*	*x*	1/2	0	$0 < x < 1/2$
16*k*	*Q*		*P*-*N*	*x*	1/2-*x*	1/4	$0 < x < 1/4$

4*e*=(Γ-*Z*)+(Z_0-*M*), $\eta = \frac{1}{4}\left(1 + \frac{c^2}{a^2}\right)$.

Table 40. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $I4/m$ and $c < a$. G^* is $(I4/m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2*a*	Γ	Γ	Γ	0	0	0	
2*b*	*M*	*M*	*M*	1/2	1/2	0	
4*c*	*X*	*X*	*X*	0	1/2	0	
4*d*	*P*	*P*	*P*	0	1/2	1/4	
4*e*	Λ		Γ-*Z*	0	0	*z*	$0 < z < \eta$
4*e*	*V*		*M*-Z_0	1/2	1/2	*z*	$0 < z < 1/2 - \eta$
4*e*	*Z*	*Z*	Z	0	0	η	
4*e*		Z_1	Z_0	1/2	1/2	1/2-η	
8*f*	*N*	*N*	*N*	1/4	1/4	1/4	
8*g*	*W*		*X*-*P*	0	1/2	*z*	$0 < z < 1/4$

4*e*=(Γ-*Z*)+(Z_0-*M*), $\eta = \frac{1}{4}\left(1 + \frac{c^2}{a^2}\right)$.

Table 41. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $I4/mmm$ and $c > a$. G^* is $(I4/mmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2*a*	Γ	Γ	Γ	0	0	0	
2*b*	*M*	*Z*	*M*	0	0	1/2	
4*c*	*X*	*X*	*X*	0	1/2	0	
4*d*	*P*	*P*	*P*	0	1/2	1/4	
4*e*	Λ		Γ-*M*	0	0	*z*	$0 < z < 1/2$
8*f*	*N*	*N*	*N*	1/4	1/4	1/4	
8*g*	*W*		*X*-*P*	0	1/2	*z*	$0 < z < 1/4$
8*h*	Σ		Γ-S_0	*x*	*x*	0	$0 < x < \eta$
8*h*	*F*		*M*-*S*	*x*	*x*	1/2	$0 < x < 1/2 - \eta$
8*h*	S_0	Σ	S_0	η	η	0	
8*h*	*S*	Σ_1	*S*	1/2-η	1/2-η	1/2	
8*i*	Δ		Γ-*X*	0	*y*	0	$0 < y < 1/2$
8*j*	*Y*		*X*-*R*	*x*	1/2	0	$0 < x < \zeta$
8*j*	*U*		*M*-*G*	0	*y*	1/2	$0 < y < 1/2 - \zeta$
8*j*	*R*	*Y*	*R*	ζ	1/2	0	
8*j*	*G*	Y_1	*G*	0	1/2-ζ	1/2	
16*k*	*Q*		*P*-*N*	*x*	1/2-*x*	1/4	$0 < x < 1/4$

8*h*=(Γ-S_0)+(*S*-*M*), 8*j*=(*X*-*R*)+(*G*-*M*), $\eta = \frac{1}{4}\left(1 + \frac{a^2}{c^2}\right)$, $\zeta = \frac{a^2}{2c^2}$.

Table 42. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $I4/m$ and $c > a$. G^* is $(I4/m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2a	Γ	Γ	Γ	0	0	0	
2b	M	Z	M	0	0	1/2	
4c	X	X	X	0	1/2	0	
4d	P	P	P	0	1/2	1/4	
4e	Λ		Γ-M	0	0	z	$0 < z < 1/2$
8f	N	N	N	1/4	1/4	1/4	
8g	W		X-P	0	1/2	z	$0 < z < 1/4$
(8h)		Σ	S_0	η	η	0	
(8h)		Σ_1	S	1/2-η	1/2-η	1/2	
(8h)		Y	R	ζ	1/2	0	
(8h)		Y_1	G	0	1/2-ζ	1/2	

$\eta = \frac{1}{4}\left(1 + \frac{a^2}{c^2}\right)$, $\zeta = \frac{a^2}{2c^2}$.

Table 43. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is *Pmmm*. SC labels are for $a < b < c$. G^* is $(Pmmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1*a*	Γ	Γ	Γ	0	0	0	
1*b*	*X*	*X*	*X*	1/2	0	0	
1*c*	*Z*	*Z*	*Z*	0	0	1/2	
1*d*	*U*	*U*	*U*	1/2	0	1/2	
1*e*	*Y*	*Y*	*Y*	0	1/2	0	
1*f*	*S*	*S*	*S*	1/2	1/2	0	
1*g*	*T*	*T*	*T*	0	1/2	1/2	
1*h*	*R*	*R*	*R*	1/2	1/2	1/2	
2*i*	Σ		Γ-*X*	*x*	0	0	$0 < x < 1/2$
2*j*	*A*		*Z-U*	*x*	0	1/2	$0 < x < 1/2$
2*k*	*C*		*Y-S*	*x*	1/2	0	$0 < x < 1/2$
2*l*	*E*		*T-R*	*x*	1/2	1/2	$0 < x < 1/2$
2*m*	Δ		Γ-*Y*	0	*y*	0	$0 < y < 1/2$
2*n*	*B*		*Z-T*	0	*y*	1/2	$0 < y < 1/2$
2*o*	*D*		*X-S*	1/2	*y*	0	$0 < y < 1/2$
2*p*	*P*		*U-R*	1/2	*y*	1/2	$0 < y < 1/2$
2*q*	Λ		Γ-*Z*	0	0	*z*	$0 < z < 1/2$
2*r*	*H*		*Y-T*	0	1/2	*z*	$0 < z < 1/2$
2*s*	*G*		*X-U*	1/2	0	*z*	$0 < z < 1/2$
2*t*	*Q*		*S-R*	1/2	1/2	*z*	$0 < z < 1/2$

Table 44. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is *Fmmm* and $a^{-2} > b^{-2} + c^{-2}$. G^* is $(Immm)^*$. SC labels are for $a < b < c$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
$2a$	Γ	Γ	Γ	0	0	0	
$2b$	T	T	T	0	1/2	1/2	
$2c$	Z	Z	Z	0	0	1/2	
$2d$	Y	Y	Y	0	1/2	0	
$4e$	Σ		Γ-Σ_0	x	0	0	$0 < x < \eta$
$4e$	U		T-U_0	x	1/2	1/2	$0 < x < 1/2 - \eta$
$4e$	Σ_0	X	Σ_0	η	0	0	
$4e$	U_0	X_1	U_0	1/2-η	1/2	1/2	
$4f$	A		Z-A_0	x	0	1/2	$0 < x < \zeta$
$4f$	C		Y-C_0	x	1/2	0	$0 < x < 1/2 - \zeta$
$4f$	A_0	A	A_0	ζ	0	1/2	
$4f$	C_0	A_1	C_0	1/2-ζ	1/2	0	
$4g$	Δ		Γ-Y	0	y	0	$0 < y < 1/2$
$4h$	B		Z-T	0	y	1/2	$0 < y < 1/2$
$4i$	Λ		Γ-Z	0	0	z	$0 < z < 1/2$
$4j$	H		Y-T	0	1/2	z	$0 < z < 1/2$
$8k$	L	L	L	1/4	1/4	1/4	

$4e$=(Γ-Σ_0)+(U_0-T), $4f$=(Z-A_0)+(C_0-Y), $\zeta = \frac{1}{4}\left(1 + \frac{a^2}{b^2} - \frac{a^2}{c^2}\right)$, $\eta = \frac{1}{4}\left(1 + \frac{a^2}{b^2} + \frac{a^2}{c^2}\right)$.

Table 45. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is *Fmmm* and $c^{-2} > a^{-2} + b^{-2}$. G^* is $(Immm)^*$. SC labels are for $c < a < b$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2*a*	Γ	Γ	Γ	0	0	0	
2*b*	T	Y	T	1/2	0	0	
2*c*	Z	T	Z	1/2	1/2	0	
2*d*	Y	Z	Y	0	1/2	0	
4*e*	Σ		Γ-T	x	0	0	$0 < x < 1/2$
4*f*	C		Y-Z	x	1/2	0	$0 < x < 1/2$
4*g*	Δ		Γ-Y	0	y	0	$0 < y < 1/2$
4*h*	D		T-Z	1/2	y	0	$0 < y < 1/2$
4*i*	Λ		Γ-Λ_0	0	0	z	$0 < z < \eta$
4*i*	Q		Z-Q_0	1/2	1/2	z	$0 < z < 1/2 - \eta$
4*i*	Λ_0	X	Λ_0	0	0	η	
4*i*	Q_0	X_1	Q_0	1/2	1/2	1/2-η	
4*j*	G		T-G_0	1/2	0	z	$0 < z < 1/2 - \zeta$
4*j*	H		Y-H_0	0	1/2	z	$0 < z < \zeta$
4*j*	G_0	A_1	G_0	1/2	0	1/2-ζ	
4*j*	H_0	A	H_0	0	1/2	ζ	
8*k*	L	L	L	1/4	1/4	1/4	

4*i*=(Γ-Λ_0)+(Q_0-Z), 4*j*=(Y-H_0)+(G_0-T), $\zeta = \frac{1}{4}\left(1 + \frac{c^2}{a^2} - \frac{c^2}{b^2}\right)$, $\eta = \frac{1}{4}\left(1 + \frac{c^2}{a^2} + \frac{c^2}{b^2}\right)$.

Table 46. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is *Fmmm* and a^{-2}, b^{-2}, and c^{-2} are edges of a triangle. G^* is $(Immm)^*$. SC labels are for $a < b < c$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\text{ITA}x}$	$k_{\text{ITA}y}$	$k_{\text{ITA}z}$	
2*a*	Γ	Γ	Γ	0	0	0	
2*b*	*T*	*X*	*T*	1/2	0	0	
2*c*	*Z*	*Z*	*Z*	0	0	1/2	
2*d*	*Y*	*Y*	*Y*	0	1/2	0	
4*e*	Σ		Γ-*T*	*x*	0	0	$0 < x < 1/2$
4*f*	*A*		*Z*-A_0	*x*	0	1/2	$0 < x < \eta$
4*f*	*C*		*Y*-C_0	*x*	1/2	0	$0 < x < 1/2-\eta$
4*f*	A_0	C_1	A_0	η	0	1/2	
4*f*	C_0	*C*	C_0	1/2-η	1/2	0	
4*g*	Δ		Γ-*Y*	0	*y*	0	$0 < y < 1/2$
4*h*	*B*		*Z*-B_0	0	*y*	1/2	$0 < y < \delta$
4*h*	*D*		*T*-D_0	1/2	*y*	0	$0 < y < 1/2-\delta$
4*h*	B_0	D_1	B_0	0	δ	1/2	
4*h*	D_0	*D*	D_0	1/2	1/2-δ	0	
4*i*	Λ		Γ-*Z*	0	0	*z*	$0 < z < 1/2$
4*j*	*G*		*T*-G_0	1/2	0	*z*	$0 < z < \phi$
4*j*	*H*		*Y*-H_0	0	1/2	*z*	$0 < z < 1/2-\phi$
4*j*	G_0	H_1	G_0	1/2	0	ϕ	
4*j*	H_0	*H*	H_0	0	1/2	1/2-ϕ	
8*k*	*L*	*L*	*L*	1/4	1/4	1/4	

4*f*=(*Z*-A_0)+(C_0-*Y*), 4*h*=(*Z*-B_0)+(D_0-*T*), 4*j*=(*T*-G_0)+(H_0-*Y*), $\eta = \frac{1}{4}\left(1+\frac{a^2}{b^2}-\frac{a^2}{c^2}\right)$,

$\delta = \frac{1}{4}\left(1+\frac{b^2}{a^2}-\frac{b^2}{c^2}\right)$, $\phi = \frac{1}{4}\left(1+\frac{c^2}{b^2}-\frac{c^2}{a^2}\right)$.

Table 47. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Immm$ and c largest. G^* is $(Fmmm)^*$. SC labels are for $a < b < c$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
4a	Γ	Γ	Γ	0	0	0	
4b	X	Z	X	0	0	1/2	
8c	S	S	S	0	1/4	1/4	
8d	R	R	R	1/4	0	1/4	
8e	T	T	T	1/4	1/4	0	
8f	W	W	W	1/4	1/4	1/4	
8g	Σ		Γ-Σ_0	x	0	0	$0 < x < \zeta$
8g	F		X-F_2	x	0	1/2	$0 < x < 1/2 - \zeta$
8g	Σ_0	X	Σ_0	ζ	0	0	
8g	F_2	X_1	F_2	1/2-ζ	0	1/2	
8h	Δ		Γ-Y_0	0	y	0	$0 < y < \eta$
8h	U		X-U_0	0	y	1/2	$0 < y < 1/2 - \eta$
8h	Y_0	Y	Y_0	0	η	0	
8h	U_0	Y_1	U_0	0	1/2-η	1/2	
8i	Λ		Γ-X	0	0	z	$0 < z < 1/2$
16j	P		T-W	1/4	1/4	z	$0 < z < 1/4$
16k	Q		R-W	1/4	y	1/4	$0 < y < 1/4$
16l	D		S-W	x	1/4	1/4	$0 < x < 1/4$
(16o)	L_0	L	L_0	ζ	1/2-η	0	
(16o)	M_0	L_1	M_0	1/2-ζ	η	0	
(16o)	J_0	L_2	J_0	1/2-ζ	1/2-η	1/2	

8g=(Γ-Σ_0)+(F_2-X), 8h=(Γ-Y_0)+(U_0-X), $\zeta = \frac{1}{4}\left(1 + \frac{a^2}{c^2}\right)$, $\eta = \frac{1}{4}\left(1 + \frac{b^2}{c^2}\right)$.

Table 48. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is *Immm* and a largest. G^* is $(Fmmm)^*$. SC labels are for $b < c < a$.

Label				$\mathbf{k}$-vector coefficients			
Wyckoff	BCS	SC	New	$k_{\text{ITA}x}$	$k_{\text{ITA}y}$	$k_{\text{ITA}z}$	Range
4*a*		Γ	Γ	0	0	0	
4*b*		Z	X	1/2	0	0	
8*c*		T	S	0	1/4	1/4	
8*d*		S	R	1/4	0	1/4	
8*e*		R	T	1/4	1/4	0	
8*f*		W	W	1/4	1/4	1/4	
8*g*			Γ-X	x	0	0	$0 < x < 1/2$
8*h*			Γ-Y_0	0	y	0	$0 < y < \zeta$
8*h*			X-U_2	1/2	y	0	$0 < y < 1/2 - \zeta$
8*h*		X	Y_0	0	ζ	0	
8*h*		X_1	U_2	1/2	1/2-ζ	0	
8*i*			Γ-Λ_0	0	0	z	$0 < z < \eta$
8*i*			X-G_2	1/2	0	z	$0 < z < 1/2 - \eta$
8*i*		Y	Λ_0	0	0	η	
8*i*		Y_1	G_2	1/2	0	1/2-η	
16*j*			R-W	1/4	1/4	z	$0 < z < 1/4$
16*k*			S-W	1/4	y	1/4	$0 < y < 1/4$
16*l*			T-W	x	1/4	1/4	$0 < x < 1/4$
(16*m*)		L	K	0	ζ	1/2-η	
(16*m*)		L_1	K_2	0	1/2-ζ	η	
(16*m*)		L_2	K_4	1/2	1/2-ζ	1/2-η	

8*h*=(Γ-Y_0)+(U_2-X), 8*i*=(Γ-Λ_0)+(G_2-X), $\zeta = \frac{1}{4}\left(1+\frac{b^2}{a^2}\right)$, $\eta = \frac{1}{4}\left(1+\frac{c^2}{a^2}\right)$.

Table 49. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is *Immm* and b largest. G^* is $(Fmmm)^*$. SC labels are for $c < a < b$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
4*a*	Γ	Γ	Γ	0	0	0	
4*b*	X	Z	X	0	1/2	0	
8*c*	S	R	S	0	1/4	1/4	
8*d*	R	T	R	1/4	0	1/4	
8*e*	T	S	T	1/4	1/4	0	
8*f*	W	W	W	1/4	1/4	1/4	
8*g*	Σ		Γ-Σ_0	x	0	0	$0 < x < \eta$
8*g*	F		X-F_0	x	1/2	0	$0 < x < 1/2 - \eta$
8*g*	Σ_0	Y	Σ_0	η	0	0	
8*g*	F_0	Y_1	F_0	1/2-η	1/2	0	
8*h*	Δ		Γ-X	0	y	0	$0 < y < 1/2$
8*i*	Λ		Γ-Λ_0	0	0	z	$0 < z < \zeta$
8*i*	G		X-G_0	0	1/2	z	$0 < z < 1/2 - \zeta$
8*i*	Λ_0	X	Λ_0	0	0	ζ	
8*i*	G_0	X_1	G_0	0	1/2	1/2-ζ	
16*j*	P		T-W	1/4	1/4	z	$0 < z < 1/4$
16*k*	Q		R-W	1/4	y	1/4	$0 < y < 1/4$
16*l*	D		S-W	x	1/4	1/4	$0 < x < 1/4$
(16*n*)	V_0	L	V_0	1/2-η	0	ζ	
(16*n*)	H_0	L_1	H_0	η	0	1/2-ζ	
(16*n*)		L_2	H_2	1/2-η	1/2	1/2-ζ	

8*g*=(Γ-Σ_0)+(F_0-X), 8*i*=(Γ-Λ_0)+(G_0-X), $\zeta = \frac{1}{4}\left(1+\frac{c^2}{b^2}\right)$, $\eta = \frac{1}{4}\left(1+\frac{a^2}{b^2}\right)$.

Table 50. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Cmmm$ and $a < b$ if oC or $b < c$ if oA. G^* is $(Cmmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2a	Γ	Γ	Γ	0	0	0	
2b	Y	Y	Y	0	1/2	0	
2c	T	T	T	0	1/2	1/2	
2d	Z	Z	Z	0	0	1/2	
4e	S	S	S	1/4	1/4	0	
4f	R	R	R	1/4	1/4	1/2	
4g	Σ		Γ-Σ_0	x	0	0	$0 < x < \zeta$
4g	C		Y-C_0	x	1/2	0	$0 < x < 1/2 - \zeta$
4g	Σ_0	X	Σ_0	ζ	0	0	
4g	C_0	X_1	C_0	1/2-ζ	1/2	0	
4h	A		Z-A_0	x	0	1/2	$0 < x < \zeta$
4h	E		T-E_0	x	1/2	1/2	$0 < x < 1/2 - \zeta$
4h	A_0	A	A_0	ζ	0	1/2	
4h	E_0	A_1	E_0	1/2-ζ	1/2	1/2	
4i	Δ		Γ-Y	0	y	0	$0 < y < 1/2$
4j	B		Z-T	0	y	1/2	$0 < y < 1/2$
4k	Λ		Γ-Z	0	0	z	$0 < z < 1/2$
4l	H		Y-T	0	1/2	z	$0 < z < 1/2$
8m	D		S-R	1/4	1/4	z	$0 < z < 1/2$

4g=(Γ-Σ_0)+(C_0-Y), 4h=(Z-A_0)+(E_0-T), $\zeta = \frac{1}{4}\left(1 + \frac{a^2}{b^2}\right)$ (oC) or $\zeta = \frac{1}{4}\left(1 + \frac{b^2}{c^2}\right)$ (oA).

Table 51. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $Cmmm$ and $a > b$ if oC or $b > c$ if oA. G^* is $(Cmmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2a	Γ	Γ	Γ	0	0	0	
2b	Y	Y	Y	1/2	0	0	
2c	T		T	1/2	0	1/2	
2c		T	T_2	1/2	0	-1/2	
2d	Z		Z	0	0	1/2	
2d		Z	Z_2	0	0	-1/2	
4e	S	S	S	1/4	1/4	0	
4f	R		R	1/4	1/4	1/2	
4f		R	R_2	1/4	1/4	-1/2	
4g	Σ		Γ-Y	x	0	0	$0 < x < 1/2$
4h	A		Z-T	x	0	1/2	$0 < x < 1/2$
4i	Δ		Γ-Δ_0	0	y	0	$0 < y < \zeta$
4i	F		Y-F_0	1/2	y	0	$0 < y < 1/2 - \zeta$
4i	Δ_0	X	Δ_0	0	ζ	0	
4i	F_0	X_1	F_0	1/2	1/2-ζ	0	
4j	B		Z-B_0	0	y	1/2	$0 < y < \zeta$
4j	G		T-G_0	1/2	y	1/2	$0 < y < 1/2 - \zeta$
4j	B_0		B_0	0	ζ	1/2	
4j		A	B_2	0	ζ	-1/2	
4j	G_0		G_0	1/2	1/2-ζ	1/2	
4j		A_1	G_2	1/2	1/2-ζ	-1/2	
4k	Λ		Γ-Z	0	0	z	$0 < z < 1/2$
4l	H		Y-T	1/2	0	z	$0 < z < 1/2$
8m	D		S-R	1/4	1/4	z	$0 < z < 1/2$

4i=(Γ-Δ_0)+(F_0-Y), 4j=(Z-B_0)+(G_0-T), $\zeta = \frac{1}{4}\left(1+\frac{b^2}{a^2}\right)$ (oC) or $\zeta = \frac{1}{4}\left(1+\frac{c^2}{b^2}\right)$ (oA).

Table 52. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P6/mmm$. G^* is $(P6/mmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1*a*	Γ	Γ	Γ	0	0	0	
1*b*	*A*	*A*	*A*	0	0	1/2	
2*c*	*K*	*K*	*K*	2/3	1/3	0	
2*d*	*H*	*H*	*H*	2/3	1/3	1/2	
2*e*	Δ		Γ-*A*	0	0	*z*	$0 < z < 1/2$
3*f*	*M*	*M*	*M*	1/2	0	0	
3*g*	*L*	*L*	*L*	1/2	0	1/2	
4*h*	*P*		*K*-*H*	2/3	1/3	*z*	$0 < z < 1/2$
6*i*	*U*		*M*-*L*	1/2	0	*z*	$0 < z < 1/2$
6*j*	Σ		Γ-*M*	*x*	0	0	$0 < x < 1/2$
6*k*	*R*		*A*-*L*	*x*	0	1/2	$0 < x < 1/2$
6*l*	Λ		Γ-*K*	*x*	*x*/2	0	$0 < x < 2/3$
6*l*	*T*		*M*-*K*	*x*+1/2	2*x*	0	$0 < x < 1/6$
6*m*	*Q*		*A*-*H*	*x*	*x*/2	1/2	$0 < x < 2/3$
6*m*	*S*		*L*-*H*	*x*+1/2	2*x*	1/2	$0 < x < 1/6$

6*l*=(Γ-*K*)+(*K*-*M*), 6*m*=(*A*-*H*)+(*H*-*L*).

Table 53. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P6/m$. G^* is $(P6/mmm)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1*a*	Γ	Γ	Γ	0	0	0	
1*b*	*A*	*A*	*A*	0	0	1/2	
2*c*	*K*	*K*	*K*	2/3	1/3	0	
2*d*	*H*	*H*	*H*	2/3	1/3	1/2	
2*e*	Δ		Γ-*A*	0	0	z	$0 < z < 1/2$
3*f*	*M*	*M*	*M*	1/2	0	0	
3*g*	*L*	*L*	*L*	1/2	0	1/2	
4*h*	*P*		*K*-*H*	2/3	1/3	z	$0 < z < 1/2$
6*i*	*U*		*M*-*L*	1/2	0	z	$0 < z < 1/2$

Table 54. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P\bar{3}m1$. G^* is $(P\bar{3}1m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1a	Γ	Γ	Γ	0	0	0	
1b	A	A	A	0	0	1/2	
2c	K	K	K	2/3	1/3	0	
2d	H	H	H	2/3	1/3	1/2	
2e	Δ		Γ-A	0	0	z	$0 < z < 1/2$
3f	M	M	M	1/2	0	0	
3g	L	L	L	1/2	0	1/2	
4h	P		K-H	2/3	1/3	z	$0 < z < 1/2$
6i	Λ		Γ-K	x	x/2	0	$0 < x < 2/3$
6i	T		M-K	x+1/2	2x	0	$0 < x < 1/6$
6j	Q		A-H	x	x/2	1/2	$0 < x < 2/3$
6j	S		L-H	x+1/2	2x	1/2	$0 < x < 1/6$

6i=(Γ-K)+(K-M), 6j=(A-H)+(H-L).

Table 55. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P\bar{3}1m$. G^* is $(P\bar{3}m1)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1*a*	Γ	Γ	Γ	0	0	0	
1*b*	*A*	*A*	*A*	0	0	1/2	
2*c*	Δ		Γ-*A*	0	0	*z*	$0<z<1/2$
2*d*	*P*		*K*-*H*	2/3	1/3	*z*	$0<z<1/2$
2*d*	*PA*		H_2-*K*	2/3	1/3	*z*	$-1/2<z<0$
2*d*	*K*	*K*	*K*	2/3	1/3	0	
2*d*	*H*	*H*	*H*	2/3	1/3	1/2	
2*d*			H_2	2/3	1/3	-1/2	
3*e*	*M*	*M*	*M*	1/2	0	0	
3*f*	*L*	*L*	*L*	1/2	0	1/2	
6*g*	Σ		Γ-*M*	*x*	0	0	$0<x<1/2$
6*h*	*R*		*A*-*L*	*x*	0	1/2	$0<x<1/2$

2*d*=(H_2-*K*)+(*K*-*H*).

Table 56. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P\bar{3}$. G^* is $(P\bar{3})^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1*a*	Γ	Γ	Γ	0	0	0	
1*b*	*A*	*A*	*A*	0	0	1/2	
2*c*	Δ		Γ-*A*	0	0	*z*	$0 < z < 1/2$
2*d*	*P*		*K*-*H*	2/3	1/3	*z*	$0 < z < 1/2$
2*d*	*PA*		H_2-*K*	2/3	1/3	*z*	$-1/2 < z < 0$
2*d*	*K*	*K*	*K*	2/3	1/3	0	
2*d*	*H*	*H*	*H*	2/3	1/3	1/2	
2*d*			H_2	2/3	1/3	-1/2	
3*e*	*M*	*M*	*M*	1/2	0	0	
3*f*	*L*	*L*	*L*	1/2	0	1/2	

2*d*=(H_2-*K*)+(*K*-*H*).

Table 57. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $R\bar{3}m$ and $\sqrt{3}a < \sqrt{2}c$. G^* is $(R\bar{3}m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
3a	Γ	Γ	Γ	0	0	0	
3b	T	Z	T	0	0	1/2	
6c	Λ		Γ-T	0	0	z	$0 < z < 1/2$
9d	L	L	L	1/3	1/6	1/6	
9d			L_2	1/6	-1/6	-1/6	
9d		L_1	L_4	1/6	1/3	-1/6	
9e	FB		F	1/6	-1/6	1/3	
9e		F	F_2	1/6	1/3	1/3	
18f	Σ		Γ-S_0	x	0	0	$0 < x < 1/3 + \delta$
18f	Q		F-S_2	1/6+x	-1/6+x	1/3	$0 < x < 1/6 - \delta$
18f	S_0		S_0	1/3+δ	0	0	
18f			S_2	1/3-δ	-δ	1/3	
18f		X	S_4	1/3+δ	1/3+δ	0	
18f		Q	S_6	1/3-δ	1/3	1/3	
18g	Y		L-H_0	1/3	y	1/6	$-2\delta < y < 1/6$
18g	B		T-H_2	x	0	1/2	$0 < x < 1/3 - 2\delta$
18g	H_0		H_0	1/3	-2δ	1/6	
18g			H_2	1/3-2δ	0	1/2	
18g		B	H_4	1/3-2δ	1/3-2δ	1/2	
18g		B_1	H_6	1/3	1/3+2δ	1/6	
(18h)	M_0		M_0	1/6+δ	-1/6-δ	1/6	
(18h)	M_2		M_2	1/6-δ	-1/6+δ	1/2	
(18h)		P	M_4	1/3-2δ	1/6-δ	1/2	
(18h)		P_1	M_6	1/6-δ	1/3-2δ	1/2	
(18h)		P_2	M_8	1/6+δ	1/3+2δ	1/6	

18f=(Γ-S_0)+(S_2-F), 18g=(L-H_0)+(H_2-T), $\delta = \dfrac{a^2}{4c^2}$.

Table 58. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $R\bar{3}$ and $\sqrt{3}a < \sqrt{2}c$. G^* is $(R\bar{3})^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
3*a*	Γ	Γ	Γ	0	0	0	
3*b*	*T*	*Z*	*T*	0	0	1/2	
6*c*	Λ		Γ-*T*	0	0	*z*	$0 < z < 1/2$
9*d*	*L*	*L*	*L*	1/3	1/6	1/6	
9*d*			L_2	1/6	-1/6	-1/6	
9*d*		L_1	L_4	1/6	1/3	-1/6	
9*e*	*FB*		*F*	1/6	-1/6	1/3	
9*e*		*F*	F_2	1/6	1/3	1/3	
[18*f*]		*X*	S_4	1/3+δ	1/3+δ	0	
[18*f*]		*Q*	S_6	1/3-δ	1/3	1/3	
[18*f*]		*B*	H_4	1/3-2δ	1/3-2δ	1/2	
[18*f*]		B_1	H_6	1/3	1/3+2δ	1/6	
[18*f*]		*P*	M_4	1/3-2δ	1/6-δ	1/2	
[18*f*]		P_1	M_6	1/6-δ	1/3-2δ	1/2	
[18*f*]		P_2	M_8	1/6+δ	1/3+2δ	1/6	

$\delta = \dfrac{a^2}{4c^2}$.

Table 59. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $R\bar{3}m$ and $\sqrt{3}a > \sqrt{2}c$. G^* is $(R\bar{3}m)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
3a	Γ	Γ	Γ	0	0	0	
3b	T	Z	T	1/3	-1/3	1/6	
6c	P		P_0-T	1/3	-1/3	z	$1/6-2\zeta < z < 1/6$
6c	Λ		Γ-P_2	0	0	z	$0 < z < 1/2-2\zeta$
6c	P_0		P_0	1/3	-1/3	1/6-2ζ	
6c	P_2	Q	P_2	0	0	1/2-2ζ	
6c		Q_1	R_0	2/3	1/3	-1/6+2ζ	
6c		P	M	1/3	-1/3	1/6-ζ	
6c		P_1	M_2	2/3	1/3	-1/6+ζ	
9d	L	L	L	1/3	1/6	1/6	
9e	FA	F	F	1/2	0	0	
18f	Σ		Γ-F	x	0	0	$0 < x < 1/2$
18g	Y		T-L	1/3	y	1/6	$-1/3 < y < 1/6$

6c=(Γ-P_2)+(P_0-T), $\zeta = \frac{1}{6} - \frac{c^2}{9a^2}$.

Table 60. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $R\bar{3}$ and $\sqrt{3}a > \sqrt{2}c$. G^* is $(R\bar{3})^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
3*a*	Γ	Γ	Γ	0	0	0	
3*b*	*T*	*Z*	*T*	1/3	-1/3	1/6	
6*c*	*P*		P_0-T	1/3	-1/3	z	$1/6-2\zeta < z < 1/6$
6*c*	Λ		Γ-P_2	0	0	z	$0 < z < 1/2-2\zeta$
6*c*	P_0		P_0	1/3	-1/3	1/6-2ζ	
6*c*	P_2	*Q*	P_2	0	0	1/2-2ζ	
6*c*		Q_1	R_0	2/3	1/3	-1/6+2ζ	
6*c*		*P*	*M*	1/3	-1/3	1/6-ζ	
6*c*		P_1	M_2	2/3	1/3	-1/6+ζ	
9*d*	*L*	*L*	*L*	1/3	1/6	1/6	
9*e*	*FA*	*F*	*F*	1/2	0	0	

6*c*=(Γ-P_2)+(P_0-*T*), $\zeta = \dfrac{1}{6} - \dfrac{c^2}{9a^2}$.

Table 61. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P2/m$ (=$P12/m1$). SC labels are for $a < c$. G^* is $(P12/m1)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
1a	Γ	Γ	Γ	0	0	0	
1b	Z	Z	Z	0	1/2	0	
1c	B	Y	B	0	0	1/2	
1c		Y_1	B_2	0	0	-1/2	
1d	Y		Y	1/2	0	0	
1d		X	Y_2	-1/2	0	0	
1e	C		C	1/2	1/2	0	
1e		A	C_2	-1/2	1/2	0	
1f	D	D	D	0	1/2	1/2	
1f		D_1	D_2	0	1/2	-1/2	
1g	A	C	A	-1/2	0	1/2	
1h	E	E	E	-1/2	1/2	1/2	
2i	Λ		Γ-Z	0	y	0	$0 < y < 1/2$
2j	W		Y-C	1/2	y	0	$0 < y < 1/2$
2j			Y_2-C_2	-1/2	y	0	$0 < y < 1/2$
2k	V		B-D	0	y	1/2	$0 < y < 1/2$
2l	U		A-E	-1/2	y	1/2	$0 < y < 1/2$
(2m)		H	H	-η	0	1-ν	
(2m)		H_1	H_2	-1+η	0	ν	
(2m)		H_2	H_4	-η	0	-ν	
(2n)		M	M	-η	1/2	1-ν	
(2n)		M_1	M_2	-1+η	1/2	ν	
(2n)		M_2	M_4	-η	1/2	-ν	

$\eta = \dfrac{1+(a/c)\cos\beta}{2\sin^2\beta}$, $\nu = \dfrac{1}{2} + \dfrac{\eta c\cos\beta}{a}$.

Table 62. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $C2/m$ (=$C12/m1$) and $b < a\sin\beta$. G^* is $(C12/m1)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2*a*	Γ	Γ	Γ	0	0	0	
2*b*	*Y*(ex)			0	1/2	0	
2*b*		*Y*	Y_2	-1/2	0	0	
2*b*		Y_1	Y_4	1/2	0	0	
2*c*	*A*	*Z*	*A*	0	0	1/2	
2*d*	*M*(ex)			0	1/2	1/2	
2*d*		*L*	M_2	-1/2	0	1/2	
4*e*	*V*	N_1	*V*	1/4	1/4	0	
4*e*		*N*	V_2	-1/4	1/4	0	
4*f*	*L*(ex)			1/4	1/4	1/2	
4*f*		*M*	L_2	-1/4	1/4	1/2	
4*g*	Λ(ex)			0	*y*	0	$0<y<1/2$
4*g*			Γ-*C*	0	*y*	0	$0<y<1-\psi$
4*g*			Y_2-N_2	-1/2	*y*	0	$0<y<-1/2+\psi$
4*g*		*X*	*C*	0	1-ψ	0	
4*g*		X_1	C_2	-1/2	-1/2+ψ	0	
4*g*		X_2	C_4	1/2	-1/2+ψ	0	
4*h*	*U*(ex)			0	*y*	1/2	$0<y<1/2$
4*h*			*A*-D_2	0	*y*	1/2	$0<y<1-\phi$
4*h*			M_2-*D*	-1/2	*y*	1/2	$0<y<-1/2+\phi$
4*h*		*I*	*D*	-1/2	-1/2+ϕ	1/2	
4*h*		I_1	D_2	0	1-ϕ	1/2	
(4*i*)		*F*	*E*	-1+ζ	0	1-η	
(4*i*)		F_1	E_2	-ζ	0	η	
(4*i*)		F_2	E_4	ζ	0	1-η	

4*g*=(Γ-*C*)+(C_2-Y_2), 4*h*=(*A*-D_2)+(*D*-M_2), $\zeta = \dfrac{2+(a/c)\cos\beta}{4\sin^2\beta}$, $\eta = \dfrac{1}{2} - \dfrac{2\zeta c\cos\beta}{a}$,

$\psi = \dfrac{3}{4} - \dfrac{b^2}{4a^2\sin^2\beta}$, $\phi = \psi - \left(\dfrac{3}{4} - \psi\right)\dfrac{a\cos\beta}{c}$.

Table 63. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $C2/m$ (=$C12/m1$) and $b > a\sin\beta$ and $-\frac{a\cos\beta}{c}+\frac{a^2\sin^2\beta}{b^2}<1$. G^* is $(C12/m1)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
$2a$	Γ	Γ	Γ	0	0	0	
$2b$	Y	X	Y	0	1/2	0	
$2c$	A	Z	A	0	0	1/2	
$2d$	M	I	M	0	1/2	1/2	
$4e$	V(ex)	N_1		1/4	1/4	0	
$4e$		N	V_2	-1/4	1/4	0	
$4f$	L(ex)			1/4	1/4	1/2	
$4f$		M	L_2	-1/4	1/4	1/2	
$4g$	Λ		Γ-Y	0	y	0	$0<y<1/2$
$4h$	U		A-M	0	y	1/2	$0<y<1/2$
($4i$)		F	F	$-1+\phi$	0	$1-\psi$	
($4i$)		F_1	F_2	$1/2-\phi$	1/2	ψ	
($4i$)		F_2	F_4	$-1/2+\phi$	1/2	$1-\psi$	
($4i$)		H	H	$-\zeta$	0	η	
($4i$)		H_1	H_2	$-1/2+\zeta$	1/2	$1-\eta$	
($4i$)		H_2	H_4	ζ	0	$1-\eta$	
($4i$)		Y	G	$-\mu$	0	δ	
($4i$)		Y_1	G_2	$-1/2+\mu$	1/2	$-\delta$	
($4i$)		Y_2	G_4	μ	0	$-\delta$	
($4i$)		Y_3	G_6	$1/2-\mu$	1/2	δ	

$\mu=\frac{1}{4}\left(1+\frac{a^2}{b^2}\right)$, $\delta=-\frac{ac\cos\beta}{2b^2}$, $\zeta=\frac{1}{4}\left(\frac{a^2}{b^2}+\frac{1+(a/c)\cos\beta}{\sin^2\beta}\right)$, $\eta=\frac{1}{2}-\frac{2\zeta c\cos\beta}{a}$, $\phi=1+\zeta-2\mu$. $\psi=\eta-2\delta$.

Table 64. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $C2/m$ (=$C12/m1$) and $b > a\sin\beta$ and $-\dfrac{a\cos\beta}{c} + \dfrac{a^2\sin^2\beta}{b^2} > 1$. G^* is $(C12/m1)^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	
2a	Γ	Γ	Γ	0	0	0	
2b	Y	X	Y	0	1/2	0	
2c	A	Z	A	0	0	1/2	
2d	M(ex)		M	0	1/2	1/2	
2d		L	M_2	-1/2	0	1/2	
4e	V	N_1	V	1/4	1/4	0	
4e		N	V_2	-1/4	1/4	0	
4f	L(ex)			1/4	1/4	1/2	
4f		M	L_2	-1/4	1/4	1/2	
4g	Λ		Γ-Y	0	y	0	$0 < y < 1/2$
4h	U(ex)			0	y	1/2	$0 < y < 1/2$
4h			A-I_2	0	y	1/2	$0 < y < 1-\rho$
4h			M_2-I	-1/2	y	1/2	$0 < y < 1/2+\rho$
4h		I	I	-1/2	-1/2+ρ	1/2	
4h		I_1	I_2	0	1-ρ	1/2	
(4i)		F	K	-ν	0	ω	
(4i)		F_1	K_2	-1+ν	0	1-ω	
(4i)		F_2	K_4	1/2-ν	1/2	ω	
(4i)		H	H	-ζ	0	η	
(4i)		H_1	H_2	-1/2+ζ	1/2	1-η	
(4i)		H_2	H_4	ζ	0	1-η	
(4i)		Y	N	-μ	0	δ	
(4i)		Y_1	N_2	-1/2+μ	1/2	-δ	
(4i)		Y_2	N_4	μ	0	-δ	
(4i)		Y_3	N_6	1/2-μ	1/2	δ	

4h=(A-I_2)+(I-M_2), $\zeta = \frac{1}{4}\left(\frac{a^2}{b^2} + \frac{1+(a/c)\cos\beta}{\sin^2\beta}\right)$, $\mu = \frac{\eta}{2} + \frac{a^2}{4b^2} + \frac{ac\cos\beta}{2b^2}$,

$\omega = \frac{c}{2a\cos\beta}\left(1 - 4\nu + \frac{a^2\sin^2\beta}{b^2}\right)$, $\eta = \frac{1}{2} - \frac{2\zeta c\cos\beta}{a}$, $\delta = -\frac{1}{4} + \frac{\omega}{2} - \frac{\zeta c\cos\beta}{a}$,

$\nu = 2\mu - \zeta$, $\rho = 1 - \frac{\zeta b^2}{a^2}$.

Table 65. Transformation matrix $\boldsymbol{M}''$ for triclinic cells.

Condition	Transformation matrix $\boldsymbol{M}''$	$\boldsymbol{M}''^{-1}$
$\lvert k_b'' k_c'' \cos k_\alpha'' \rvert$ is smallest	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
$\lvert k_c'' k_a'' \cos k_\beta'' \rvert$ is smallest	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$\lvert k_a'' k_b'' \cos k_\gamma'' \rvert$ is smallest	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 66. Transformation matrix $\boldsymbol{M}'''$ for triclinic cells.

Condition	Transformation matrix $\boldsymbol{M}'''$ $(= \boldsymbol{M}'''^{-1})$
$k'''_\alpha < 90°$, $k'''_\beta < 90°$ and $k'''_\gamma < 90°$ OR $k'''_\alpha > 90°$, $k'''_\beta > 90°$ and $k'''_\gamma > 90°$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$k'''_\alpha < 90°$, $k'''_\beta > 90°$ and $k'''_\gamma > 90°$ OR $k'''_\alpha > 90°$, $k'''_\beta < 90°$ and $k'''_\gamma < 90$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
$k'''_\alpha > 90°$, $k'''_\beta < 90°$ and $k'''_\gamma > 90$ OR $k'''_\alpha < 90°$, $k'''_\beta > 90°$ and $k'''_\gamma < 90°$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
$k'''_\alpha > 90°$, $k'''_\beta > 90°$ and $k'''_\gamma < 90°$ OR $k'''_\alpha < 90°$, $k'''_\beta < 90°$ and $k'''_\gamma > 90°$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 67. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space f when G is $P\bar{1}$ and the interaxial angles of the reciprocal "reduced" cell are all-obtuse. G^* is $(P\bar{1})^*$.

Label				$\mathbf{k}$-vector coefficients			Range
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}, k'_{\mathrm{P}x}, k_{\mathrm{R}x}$	$k_{\mathrm{ITA}y}, k'_{\mathrm{P}y}, k_{\mathrm{R}y}$	$k_{\mathrm{ITAz}}, k'_{\mathrm{Pz}}, k_{\mathrm{Rz}}$	
1a	Γ	Γ	Γ	0	0	0	
1b	Z	Z	Z	0	0	1/2	
1c	Y	Y	Y	0	1/2	0	
1d	X	X	X	1/2	0	0	
1e	V	L	V	1/2	1/2	0	
1f	U	N	U	1/2	0	1/2	
1g	T	M	T	0	1/2	1/2	
1h	R	R	R	1/2	1/2	1/2	

Table 68. Labels and $\mathbf{k}$-vector coefficients of points and lines in reciprocal space when G is $P\bar{1}$ and the interaxial angles of the reciprocal "reduced" cell are all-acute. G^* is $(P\bar{1})^*$.

Label				$\mathbf{k}$-vector coefficients			
Wyckoff	BCS	SC	New	$k_{\mathrm{ITA}x}, k'_{\mathrm{P}x}, k_{\mathrm{R}x}$	$k_{\mathrm{ITA}y}, k'_{\mathrm{P}y}, k_{\mathrm{R}y}$	$k_{\mathrm{ITA}z}, k'_{\mathrm{P}z}, k_{\mathrm{R}z}$	Range
1*a*	Γ	Γ	Γ	0	0	0	
1*b*	*Z*	*M*	*Z*	0	0	1/2	
1*c*	*Y*		*Y*	0	1/2	0	
1*c*		*X*	Y_2	0	-1/2	0	
1*d*	*X*	*Y*	*X*	1/2	0	0	
1*e*	*V*(ex)			1/2	1/2	0	
1*e*		*L*	V_2	1/2	-1/2	0	
1*f*	*U*(ex)			1/2	0	1/2	
1*f*		*Z*	U_2	-1/2	0	1/2	
1*g*	*T*(ex)			0	1/2	1/2	
1*g*		*R*	T_2	0	-1/2	1/2	
1*h*	*R*(ex)			1/2	1/2	1/2	
1*h*		*N*	R_2	-1/2	-1/2	1/2	

Table 69. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *cP*. The additional path M–X_2 is recommended for space group types $P23$, $P2_13$, $Pm\bar{3}$, $Pa\bar{3}$, and $Pn\bar{3}$ (numbers 195, 198, 200, 201, and 205, respectively).

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
R	1/2	1/2	1/2	1/2	1/2	1/2
M	1/2	1/2	0	1/2	1/2	0
X	0	1/2	0	0	1/2	0
X_1	1/2	0	0	1/2	0	0

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Recommended path: Γ–X–M–Γ–R–X | R–M (–X_1)

Table 70. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *cF*. The Additional path X–W_2 is recommended for space group types $F23$, $Fm\bar{3}$, and $Fd\bar{3}$ (numbers 196, 202, and 203, respectively).

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
X	0	1/2	0	1/2	0	1/2
L	1/4	1/4	1/4	1/2	1/2	1/2
W	1/4	1/2	0	1/2	1/4	3/4
W_2	0	1/2	1/4	3/4	1/4	1/2
K	3/8	3/8	0	3/8	3/8	3/4
U	1/8	1/2	1/8	5/8	1/4	5/8

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

Recommended path: Γ–X–U | K–Γ–L–W–X (–W_2)

Table 71. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *cI*.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
H	0	1/2	0	1/2	-1/2	1/2
P	1/4	1/4	1/4	1/4	1/4	1/4
N	1/4	1/4	0	0	0	1/2

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}.$$

Recommended path: Γ–*H*–*N*–Γ–*P*–*H* | *P*–*N*

Table 72. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *tP*.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
Z	0	0	1/2	0	0	1/2
M	1/2	1/2	0	1/2	1/2	0
A	1/2	1/2	1/2	1/2	1/2	1/2
R	0	1/2	1/2	0	1/2	1/2
X	0	1/2	0	0	1/2	0

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Recommended path: Γ–*X*–*M*–Γ–*Z*–*R*–*A*–*Z* | *X*–*R* | *M*–*A*

Table 73. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *tI* when $c < a$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
M	1/2	1/2	0	-1/2	1/2	1/2
X	0	1/2	0	0	0	1/2
P	0	1/2	1/4	1/4	1/4	1/4
Z	0	0	η	η	η	$-\eta$
Z_0	1/2	1/2	$1/2-\eta$	$-\eta$	$1-\eta$	η
N	1/4	1/4	1/4	0	1/2	0

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}, \quad \eta = \frac{1}{4}\left(1 + \frac{c^2}{a^2}\right).$$

Recommended path: Γ–*X*–*M*–Γ–*Z* | Z_0–*M* | *X*–*P*–*N*–Γ

Table 74. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *tI* when $c > a$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
M	0	0	1/2	1/2	1/2	-1/2
X	0	1/2	0	0	0	1/2
P	0	1/2	1/4	1/4	1/4	1/4
N	1/4	1/4	1/4	0	1/2	0
S_0	η	η	0	-η	η	η
S	1/2-η	1/2-η	1/2	η	1-η	-η
R	ζ	1/2	0	-ζ	ζ	1/2
G	0	1/2-ζ	1/2	1/2	1/2	-ζ

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & \bar{1} \end{pmatrix},\ \eta = \frac{1}{4}\left(1 + \frac{a^2}{c^2}\right),\ \zeta = \frac{a^2}{2c^2}.$$

Recommended path: Γ–*X*–*P*–*N*–Γ–*M*–*S* | S_0–Γ | *X*–*R* | *G*–*M*

Table 75. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oP*.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
X	1/2	0	0	1/2	0	0
Z	0	0	1/2	0	0	1/2
U	1/2	0	1/2	1/2	0	1/2
Y	0	1/2	0	0	1/2	0
S	1/2	1/2	0	1/2	1/2	0
T	0	1/2	1/2	0	1/2	1/2
R	1/2	1/2	1/2	1/2	1/2	1/2

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Recommended path: Γ–*X*–*S*–*Y*–Γ–*Z*–*U*–*R*–*T*–*Z* | *X*–*U* | *Y*–*T* | *S*–*R*

Table 76. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oF* when $a^{-2} > b^{-2} + c^{-2}$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
T	0	1/2	1/2	1	1/2	1/2
Z	0	0	1/2	1/2	1/2	0
Y	0	1/2	0	1/2	0	1/2
Σ_0	η	0	0	0	η	η
U_0	1/2-η	1/2	1/2	1	1-η	1-η
A_0	ζ	0	1/2	1/2	1/2+ζ	ζ
C_0	1/2-ζ	1/2	0	1/2	1/2-ζ	1-ζ
L	1/4	1/4	1/4	1/2	1/2	1/2

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \ \zeta = \frac{1}{4}\left(1 + \frac{a^2}{b^2} - \frac{a^2}{c^2}\right), \ \eta = \frac{1}{4}\left(1 + \frac{a^2}{b^2} + \frac{a^2}{c^2}\right).$$

Recommended path: Γ–Y–T–Z–Γ–Σ_0 | U_0–T | Y–C_0 | A_0–Z | Γ–L

Table 77. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oF* when $c^{-2} > a^{-2} + b^{-2}$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
T	1/2	0	0	0	1/2	1/2
Z	1/2	1/2	0	1/2	1/2	1
Y	0	1/2	0	1/2	0	1/2
Λ_0	0	0	η	η	η	0
Q_0	1/2	1/2	1/2-η	1-η	1-η	1
G_0	1/2	0	1/2-ζ	1/2-ζ	1-ζ	1/2
H_0	0	1/2	ζ	1/2+ζ	ζ	1/2
L	1/4	1/4	1/4	1/2	1/2	1/2

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \ \zeta = \frac{1}{4}\left(1 + \frac{c^2}{a^2} - \frac{c^2}{b^2}\right), \ \eta = \frac{1}{4}\left(1 + \frac{c^2}{a^2} + \frac{c^2}{b^2}\right).$$

Recommended path: Γ–T–Z–Y–Γ–Λ_0 | Q_0–Z | T–G_0 | H_0–Y | Γ–L

Table 78. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oF* when a^{-2}, b^{-2}, and c^{-2} are edges of a triangle.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
T	1/2	0	0	0	1/2	1/2
Z	0	0	1/2	1/2	1/2	0
Y	0	1/2	0	1/2	0	1/2
A_0	η	0	1/2	1/2	1/2+η	η
C_0	1/2-η	1/2	0	1/2	1/2-η	1-η
B_0	0	δ	1/2	1/2+δ	1/2	δ
D_0	1/2	1/2-δ	0	1/2-δ	1/2	1-δ
G_0	1/2	0	ϕ	ϕ	1/2+ϕ	1/2
H_0	0	1/2	1/2-ϕ	1-ϕ	1/2-ϕ	1/2
L	1/4	1/4	1/4	1/2	1/2	1/2

$$\boldsymbol{Q}^{-1}=\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix},\ \eta=\frac{1}{4}\left(1+\frac{a^2}{b^2}-\frac{a^2}{c^2}\right),\ \delta=\frac{1}{4}\left(1+\frac{b^2}{a^2}-\frac{b^2}{c^2}\right),\ \phi=\frac{1}{4}\left(1+\frac{c^2}{b^2}-\frac{c^2}{a^2}\right).$$

Recommended path: Γ–Y–C_0 | A_0–Z–B_0 | D_0–T–G_0 | H_0–Y | T–Γ–Z | Γ–L

Table 79. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oI* when *c* is the largest.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
X	0	0	1/2	1/2	1/2	-1/2
S	0	1/4	1/4	1/2	0	0
R	1/4	0	1/4	0	1/2	0
T	1/4	1/4	0	0	0	1/2
W	1/4	1/4	1/4	1/4	1/4	1/4
Σ_0	ζ	0	0	$-\zeta$	ζ	ζ
F_2	$1/2-\zeta$	0	1/2	ζ	$1-\zeta$	$-\zeta$
Y_0	0	η	0	η	$-\eta$	η
U_0	0	$1/2-\eta$	1/2	$1-\eta$	η	$-\eta$
L_0	ζ	$1/2-\eta$	0	$-\mu$	μ	$1/2-\delta$
M_0	$1/2-\zeta$	η	0	μ	$-\mu$	$1/2+\delta$
J_0	$1/2-\zeta$	$1/2-\eta$	1/2	$1/2-\delta$	$1/2+\delta$	$-\mu$

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1+\frac{a^2}{c^2}\right), \quad \eta = \frac{1}{4}\left(1+\frac{b^2}{c^2}\right), \quad \delta = \frac{b^2-a^2}{4c^2}, \quad \mu = \frac{a^2+b^2}{4c^2}.$$

Recommended path: Γ–X–F_2 | Σ_0–Γ–Y_0 | U_0–X | Γ–R–W–S–Γ–T–W

Table 80. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oI* when *a* is the largest.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
X	1/2	0	0	-1/2	1/2	1/2
S	0	1/4	1/4	1/2	0	0
R	1/4	0	1/4	0	1/2	0
T	1/4	1/4	0	0	0	1/2
W	1/4	1/4	1/4	1/4	1/4	1/4
Y_0	0	ζ	0	ζ	-ζ	ζ
U_2	1/2	1/2-ζ	0	-ζ	ζ	1-ζ
Λ_0	0	0	η	η	η	-η
G_2	1/2	0	1/2-η	-η	1-η	η
K	0	ζ	1/2-η	1/2-δ	-μ	μ
K_2	0	1/2-ζ	η	1/2+δ	μ	-μ
K_4	1/2	1/2-ζ	1/2-η	-μ	1/2-δ	1/2+δ

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1 + \frac{b^2}{a^2}\right), \quad \eta = \frac{1}{4}\left(1 + \frac{c^2}{a^2}\right), \quad \delta = \frac{c^2 - b^2}{4a^2}, \quad \mu = \frac{b^2 + c^2}{4a^2}.$$

Recommended path: Γ–X–U_2 | Y_0–Γ–Λ_0 | G_2–*X* | Γ–*R*–*W*–*S*–Γ–*T*–*W*

Table 81. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oI* when *b* is the largest.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
X	0	1/2	0	1/2	-1/2	1/2
S	0	1/4	1/4	1/2	0	0
R	1/4	0	1/4	0	1/2	0
T	1/4	1/4	0	0	0	1/2
W	1/4	1/4	1/4	1/4	1/4	1/4
Σ_0	η	0	0	$-\eta$	η	η
F_0	$1/2-\eta$	1/2	0	η	$-\eta$	$1-\eta$
Λ_0	0	0	ζ	ζ	ζ	$-\zeta$
G_0	0	1/2	$1/2-\zeta$	$1-\zeta$	$-\zeta$	ζ
V_0	$1/2-\eta$	0	ζ	μ	$1/2-\delta$	$-\mu$
H_0	η	0	$1/2-\zeta$	$-\mu$	$1/2+\delta$	μ
H_2	$1/2-\eta$	1/2	$1/2-\zeta$	$1/2+\delta$	$-\mu$	$1/2-\delta$

$$\boldsymbol{Q}^{-1}=\begin{pmatrix}\bar{1}&1&1\\1&\bar{1}&1\\1&1&\bar{1}\end{pmatrix},\ \zeta=\frac{1}{4}\left(1+\frac{c^2}{b^2}\right),\ \eta=\frac{1}{4}\left(1+\frac{a^2}{b^2}\right),\ \delta=\frac{a^2-c^2}{4b^2},\ \mu=\frac{c^2+a^2}{4b^2}.$$

Recommended path: Γ–X–F_0 | Σ_0–Γ–Λ_0 | G_0–*X* | Γ–*R*–*W*–*S*–Γ–*T*–*W*

Table 82. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oS* when $a < b$ if *oC* or $b < c$ if *oA*.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	k_{ITAz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
Y	0	1/2	0	-1/2	1/2	0
T	0	1/2	1/2	-1/2	1/2	1/2
Z	0	0	1/2	0	0	1/2
S	1/4	1/4	0	0	1/2	0
R	1/4	1/4	1/2	0	1/2	1/2
Σ_0	ζ	0	0	ζ	ζ	0
C_0	1/2-ζ	1/2	0	-ζ	1-ζ	0
A_0	ζ	0	1/2	ζ	ζ	1/2
E_0	1/2-ζ	1/2	1/2	-ζ	1-ζ	1/2

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1 + \frac{a^2}{b^2}\right) \ (oC) \text{ or } \ \zeta = \frac{1}{4}\left(1 + \frac{b^2}{c^2}\right) \ (oA).$$

Recommended path: Γ–*Y*–C_0 | Σ_0–Γ–*Z*–A_0 | E_0–*T*–*Y* | Γ–*S*–*R*–*Z*–*T*

Table 83. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *oS* when $a > b$ if *oC* or $b > c$ if *oA*.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
Y	1/2	0	0	1/2	1/2	0
T	1/2	0	1/2	1/2	1/2	1/2
T_2	1/2	0	-1/2	1/2	1/2	-1/2
Z	0	0	1/2	0	0	1/2
Z_2	0	0	-1/2	0	0	-1/2
S	1/4	1/4	0	0	1/2	0
R	1/4	1/4	1/2	0	1/2	1/2
R_2	1/4	1/4	-1/2	0	1/2	-1/2
Δ_0	0	ζ	0	-ζ	ζ	0
F_0	1/2	1/2-ζ	0	ζ	1-ζ	0
B_0	0	ζ	1/2	-ζ	ζ	1/2
B_2	0	ζ	-1/2	-ζ	ζ	-1/2
G_0	1/2	1/2-ζ	1/2	ζ	1-ζ	1/2
G_2	1/2	1/2-ζ	-1/2	ζ	1-ζ	-1/2

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(1+\frac{b^2}{a^2}\right) \ (oC) \text{ or } \ \zeta = \frac{1}{4}\left(1+\frac{c^2}{b^2}\right) \ (oA).$$

Recommended path: Γ–Y–F_0 | Δ_0–Γ–Z–B_0 | G_0–T–Y | Γ–S–R–Z–T

Table 84. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *hP*. Additional path K–H_2 is recommended for space group types $P3$, $P3_1$, $P3_2$, $P\bar{3}$, $P312$, $P3_112$ $P3_212$, $P31m$, P31c, $P\bar{3}1m$, and $P\bar{3}1c$ (numbers 143, 144, 145, 147, 149, 151, 153, 157, 159, 162, and 163, respectively).

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
A	0	0	1/2	0	0	1/2
K	2/3	1/3	0	1/3	1/3	0
H	2/3	1/3	1/2	1/3	1/3	1/2
H_2	2/3	1/3	-1/2	1/3	1/3	-1/2
M	1/2	0	0	1/2	0	0
L	1/2	0	1/2	1/2	0	1/2

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Recommended path: Γ–M–K–Γ–A–L–H–A | M–L | H–K(–H_2)

Table 85. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *hR* when $\sqrt{3}a < \sqrt{2}c$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
T	0	0	1/2	1/2	1/2	1/2
L	1/3	1/6	1/6	1/2	0	0
L_2	1/6	-1/6	-1/6	0	-1/2	0
L_4	1/6	1/3	-1/6	0	0	-1/2
F	1/6	-1/6	1/3	1/2	0	1/2
F_2	1/6	1/3	1/3	1/2	1/2	0
S_0	$1/3+\delta$	0	0	ν	$-\nu$	0
S_2	$1/3-\delta$	$-\delta$	1/3	$1-\nu$	0	ν
S_4	$1/3+\delta$	$1/3+\delta$	0	ν	0	$-\nu$
S_6	$1/3-\delta$	1/3	1/3	$1-\nu$	ν	0
H_0	1/3	-2δ	1/6	1/2	$-1+\eta$	$1-\eta$
H_2	$1/3-2\delta$	0	1/2	η	$1-\eta$	1/2
H_4	$1/3-2\delta$	$1/3-2\delta$	1/2	η	1/2	$1-\eta$
H_6	1/3	$1/3+2\delta$	1/6	1/2	$1-\eta$	$-1+\eta$
M_0	$1/6+\delta$	$-1/6-\delta$	1/6	ν	$-1+\eta$	ν
M_2	$1/6-\delta$	$-1/6+\delta$	1/2	$1-\nu$	$1-\eta$	$1-\nu$
M_4	$1/3-2\delta$	$1/6-\delta$	1/2	η	ν	ν
M_6	$1/6-\delta$	$1/3-2\delta$	1/2	$1-\nu$	$1-\nu$	$1-\eta$
M_8	$1/6+\delta$	$1/3+2\delta$	1/6	ν	ν	$-1+\eta$

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}, \quad \delta = \frac{a^2}{4c^2}, \quad \eta = \frac{5}{6} - 2\delta, \quad \nu = \frac{1}{3} + \delta.$$

Recommended path: Γ–T–H_2 | H_0–L–Γ–S_0 | S_2–F–Γ

Table 86. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *hR* when $\sqrt{3}a > \sqrt{2}c$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	k_{ITAz}	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	k_{Pz}
Γ	0	0	0	0	0	0
T	1/3	-1/3	1/6	1/2	-1/2	1/2
P_0	1/3	-1/3	1/6-2ζ	η	-1+η	η
P_2	0	0	1/2-2ζ	η	η	η
R_0	2/3	1/3	-1/6+2ζ	1-η	-η	-η
M	1/3	-1/3	1/6-ζ	1-ν	-ν	1-ν
M_2	2/3	1/3	-1/6+ζ	ν	-1+ν	-1+ν
L	1/3	1/6	1/6	1/2	0	0
F	1/2	0	0	1/2	-1/2	0

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}, \quad \zeta = \frac{1}{6} - \frac{c^2}{9a^2}, \quad \eta = \frac{1}{2} - 2\zeta, \quad \nu = \frac{1}{2} + \zeta .$$

Recommended path: Γ–L–T–P_0 | P_2–Γ–F

Table 87. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *mP*.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
Z	0	1/2	0	0	1/2	0
B	0	0	1/2	0	0	1/2
B_2	0	0	-1/2	0	0	-1/2
Y	1/2	0	0	1/2	0	0
Y_2	-1/2	0	0	-1/2	0	0
C	1/2	1/2	0	1/2	1/2	0
C_2	-1/2	1/2	0	-1/2	1/2	0
D	0	1/2	1/2	0	1/2	1/2
D_2	0	1/2	-1/2	0	1/2	-1/2
A	-1/2	0	1/2	-1/2	0	1/2
E	-1/2	1/2	1/2	-1/2	1/2	1/2
H	$-\eta$	0	$1-\nu$	$-\eta$	0	$1-\nu$
H_2	$-1+\eta$	0	ν	$-1+\eta$	0	ν
H_4	$-\eta$	0	$-\nu$	$-\eta$	0	$-\nu$
M	$-\eta$	1/2	$1-\nu$	$-\eta$	1/2	$1-\nu$
M_2	$-1+\eta$	1/2	ν	$-1+\eta$	1/2	ν
M_4	$-\eta$	1/2	$-\nu$	$-\eta$	1/2	$-\nu$

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \eta = \frac{1+(a/c)\cos\beta}{2\sin^2\beta}, \quad \nu = \frac{1}{2} + \frac{\eta c\cos\beta}{a}.$$

Recommended path: Γ–Z–D–B–Γ–A–E–Z–C_2–Y_2–Γ

Table 88. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for mC when $b < a\sin\beta$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\text{ITA}x}$	$k_{\text{ITA}y}$	$k_{\text{ITA}z}$	$k_{\text{P}x}$	$k_{\text{P}y}$	$k_{\text{P}z}$
Γ	0	0	0	0	0	0
Y_2	-1/2	0	0	-1/2	1/2	0
Y_4	1/2	0	0	1/2	-1/2	0
A	0	0	1/2	0	0	1/2
M_2	-1/2	0	1/2	-1/2	1/2	1/2
V	1/4	1/4	0	1/2	0	0
V_2	-1/4	1/4	0	0	1/2	0
L_2	-1/4	1/4	1/2	0	1/2	1/2
C	0	1-ψ	0	1-ψ	1-ψ	0
C_2	-1/2	-1/2+ψ	0	-1+ψ	ψ	0
C_4	1/2	-1/2+ψ	0	ψ	-1+ψ	0
D	-1/2	-1/2+ϕ	1/2	-1+ϕ	ϕ	1/2
D_2	0	1-ϕ	1/2	1-ϕ	1-ϕ	1/2
E	-1+ζ	0	1-η	-1+ζ	1-ζ	1-η
E_2	-ζ	0	η	-ζ	ζ	η
E_4	ζ	0	1-η	ζ	-ζ	1-η

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \zeta = \frac{2 + (a/c)\cos\beta}{4\sin^2\beta}, \quad \eta = \frac{1}{2} - \frac{2\zeta c\cos\beta}{a}, \quad \psi = \frac{3}{4} - \frac{b^2}{4a^2\sin^2\beta},$$

$$\phi = \psi - \left(\frac{3}{4} - \psi\right)\frac{a\cos\beta}{c}.$$

Recommended path: Γ–C | C_2–Y_2–Γ–M_2–D | D_2–A–Γ | L_2–Γ–V_2

Table 89. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *mC* when $b > a\sin\beta$ and $-\dfrac{a\cos\beta}{c}+\dfrac{a^2\sin^2\beta}{b^2}<1$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
Y	0	1/2	0	1/2	1/2	0
A	0	0	1/2	0	0	1/2
M	0	1/2	1/2	1/2	1/2	1/2
V_2	-1/4	1/4	0	0	1/2	0
L_2	-1/4	1/4	1/2	0	1/2	1/2
F	-1+ϕ	0	1-ψ	-1+ϕ	1-ϕ	1-ψ
F_2	1/2-ϕ	1/2	ψ	1-ϕ	ϕ	ψ
F_4	-1/2+ϕ	1/2	1-ψ	ϕ	1-ϕ	1-ψ
H	-ζ	0	η	-ζ	ζ	η
H_2	-1/2+ζ	1/2	1-η	ζ	1-ζ	1-η
H_4	ζ	0	1-η	ζ	-ζ	1-η
G	-μ	0	δ	-μ	μ	δ
G_2	-1/2+μ	1/2	-δ	μ	1-μ	-δ
G_4	μ	0	-δ	μ	-μ	-δ
G_6	1/2-μ	1/2	δ	1-μ	μ	δ

$$\boldsymbol{Q}^{-1}=\begin{pmatrix}1 & \bar{1} & 0\\ 1 & 1 & 0\\ 0 & 0 & 1\end{pmatrix},\quad \mu=\frac{1}{4}\left(1+\frac{a^2}{b^2}\right),\quad \delta=-\frac{ac\cos\beta}{2b^2},\quad \zeta=\frac{1}{4}\left(\frac{a^2}{b^2}+\frac{1+(a/c)\cos\beta}{\sin^2\beta}\right)$$

$$\eta=\frac{1}{2}-\frac{2\zeta c\cos\beta}{a},\quad \phi=1+\zeta-2\mu.\quad \psi=\eta-2\delta.$$

Recommended path: Γ–*Y*–*M*–*A*–Γ | L_2–Γ–V_2

Table 90. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined according to crystallographic convention for *mC* when $b > a\sin\beta$ and $-\dfrac{a\cos\beta}{c}+\dfrac{a^2\sin^2\beta}{b^2}>1$.

Label	$\mathbf{k}$-vector coefficients					
	$k_{\mathrm{ITA}x}$	$k_{\mathrm{ITA}y}$	$k_{\mathrm{ITA}z}$	$k_{\mathrm{P}x}$	$k_{\mathrm{P}y}$	$k_{\mathrm{P}z}$
Γ	0	0	0	0	0	0
Y	0	1/2	0	1/2	1/2	0
A	0	0	1/2	0	0	1/2
M_2	-1/2	0	1/2	-1/2	1/2	1/2
V	1/4	1/4	0	1/2	0	0
V_2	-1/4	1/4	0	0	1/2	0
L_2	-1/4	1/4	1/2	0	1/2	1/2
I	-1/2	$-1/2+\rho$	1/2	$-1+\rho$	ρ	1/2
I_2	0	$1-\rho$	1/2	$1-\rho$	$1-\rho$	1/2
K	$-\nu$	0	ω	$-\nu$	ν	ω
K_2	$-1+\nu$	0	$1-\omega$	$-1+\nu$	$1-\nu$	$1-\omega$
K_4	$1/2-\nu$	1/2	ω	$1-\nu$	ν	ω
H	$-\zeta$	0	η	$-\zeta$	ζ	η
H_2	$-1/2+\zeta$	1/2	$1-\eta$	ζ	$1-\zeta$	$1-\eta$
H_4	ζ	0	$1-\eta$	ζ	$-\zeta$	$1-\eta$
N	$-\mu$	0	δ	$-\mu$	μ	δ
N_2	$-1/2+\mu$	1/2	$-\delta$	μ	$1-\mu$	$-\delta$
N_4	μ	0	$-\delta$	μ	$-\mu$	$-\delta$
N_6	$1/2-\mu$	1/2	δ	$1-\mu$	μ	δ

$$\boldsymbol{Q}^{-1} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \zeta = \frac{1}{4}\left(\frac{a^2}{b^2} + \frac{1+(a/c)\cos\beta}{\sin^2\beta}\right), ,$$

$$\rho = 1 - \frac{\zeta b^2}{a^2}, \quad \eta = \frac{1}{2} - \frac{2\zeta c\cos\beta}{a}, \quad \mu = \frac{\eta}{2} + \frac{a^2}{4b^2} + \frac{ac\cos\beta}{2b^2}, \quad \nu = 2\mu - \zeta,$$

$$\omega = \frac{c}{2a\cos\beta}\left(1 - 4\nu + \frac{a^2\sin^2\beta}{b^2}\right)、 \delta = -\frac{1}{4} + \frac{\omega}{2} - \frac{\zeta c\cos\beta}{a}$$

Recommended path: Γ–A–I_2 | I–M_2–Γ–Y | L_2–Γ–V_2

Table 91. Suggested band path and **k** -vector coefficients of points and labels in reciprocal space defined for *aP* when the interaxial angles of the reciprocal "reduced" cell are all-obtuse.

Label	**k** -vector coefficients		
	$k_{\mathrm{R}x}$	$k_{\mathrm{R}y}$	$k_{\mathrm{R}z}$
Γ	0	0	0
Z	0	0	1/2
Y	0	1/2	0
X	1/2	0	0
V	1/2	1/2	0
U	1/2	0	1/2
T	0	1/2	1/2
R	1/2	1/2	1/2

Recommended path: Γ–*X* | *Y*–Γ–*Z* | *R*–Γ–*T* | *U*–Γ–*V*

Table 92. Suggested band path and $\mathbf{k}$-vector coefficients of points and labels in reciprocal space defined for *aP* when the interaxial angles of the reciprocal "reduced" cell are all-acute.

Label	$\mathbf{k}$-vector coefficients		
	k_{Rx}	k_{Ry}	k_{Rz}
Γ	0	0	0
Z	0	0	1/2
Y	0	1/2	0
Y_2	0	-1/2	0
X	1/2	0	0
V_2	1/2	-1/2	0
U_2	-1/2	0	1/2
T_2	0	-1/2	1/2
R_2	-1/2	-1/2	1/2

Recommended path: Γ–X | Y–Γ–Z | R_2–Γ–T_2 | U_2–Γ–V_2

Table 93. How to determine the first letter of the extended Bravais symbol. N is the space group number.

Crystal family	First letter	Range of N
Triclinic	a	$1 \leq N \leq 2$
Monoclinic	m	$3 \leq N \leq 15$
Orthorhombic	o	$16 \leq N \leq 74$
Tetragonal	t	$75 \leq N \leq 142$
Hexagonal	h	$143 \leq N \leq 194$
Cubic	c	$195 \leq N \leq 230$

Table 94. How to determine the third character of the extended Bravais symbol and the relevant table among Tables 69-92. N is the space group number. No definition is given if there is only one type in the Bravais symbol. *: Interaxial angles of the reciprocal reduced cells are either all-obtuse (aP2) or all-acute (aP3). Here, oF2Y does not exist, and aP1 is reserved for aP2+aP3.

Characters	Type definition	Table
cP1	$195 \le N \le 206$	69 (long path)
cP2	$207 \le N \le 230$	69 (short path)
cF1	$195 \le N \le 206$	70 (long path)
cF2	$207 \le N \le 230$	70 (short path)
cI1	--	71
tP1	--	72
tI1	$c < a$	73
tI2	$c > a$	74
oP1	--	75
oF1	$a^{-2} > b^{-2} + c^{-2}$	76
oF2	$c^{-2} > a^{-2} + b^{-2}$	77
oF3	*oF* but not oF1 nor oF2	78
oI1	c largest	79
oI2	a largest	80
oI3	b largest	81
oC1	$a < b$	82
oC2	$a > b$	83
oA1	$b < c$	82
oA2	$b > c$	83
hP1	One of $143 \le N \le 149$, N=151, N=153, N=157, $159 \le N \le 163$	84 (long path)
hP2	*hP* but not hP1	84 (short path)
hR1	$\sqrt{3}a < \sqrt{2}c$	85
hR2	$\sqrt{3}a > \sqrt{2}c$	86
mP1	--	87
mC1	$b < a \sin \beta$	88

mC2	$b > a\sin\beta$ and $-\frac{a\cos\beta}{c} + \frac{a^2\sin^2\beta}{b^2} < 1$	89
mC3	$b > a\sin\beta$ and $-\frac{a\cos\beta}{c} + \frac{a^2\sin^2\beta}{b^2} > 1$	90
aP2	Obtuse*	91
aP3	Acute*	92

Table 96. Point groups with inversion and the respective space group number range. *N* is the space group number.

Point group with inversion	Range
$\bar{1}$	N=2
$2/m$	$10 \le N \le 15$
mmm	$47 \le N \le 74$
$4/m$	$81 \le N \le 82$
$4/mmm$	$123 \le N \le 142$
$\bar{3}$	$147 \le N \le 148$
$\bar{3}$m1, $\bar{3}$1m, $\bar{3}$m	$162 \le N \le 167$
$6/m$	$175 \le N \le 176$
$6/mmm$	$191 \le N \le 194$
$m\bar{3}$	$200 \le N \le 206$
$m\bar{3}m$	$221 \le N \le 230$

Type of reciprocal cell	Basis vectors	**k**-vector coefficients
Reciprocal standard primitive	$(\mathbf{a}'^*_{\mathrm{P}} / \mathbf{b}'^*_{\mathrm{P}} / \mathbf{c}'^*_{\mathrm{P}})$	$(k'_{\mathrm{P}x}, k'_{\mathrm{P}y}, k'_{\mathrm{P}z})$
$(k'_{\mathrm{P}x}, k'_{\mathrm{P}y}, k'_{\mathrm{P}z}) = (k'_x, k'_y, k'_z)\boldsymbol{P}'$		
Reciprocal standard conventional	$(\mathbf{a}'^* / \mathbf{b}'^* / \mathbf{c}'^*)$	(k'_x, k'_y, k'_z)
$(k'_x, k'_y, k'_z) = (k_x, k_y, k_z)\boldsymbol{S}$		
Reciprocal crystallographic conventional	$(\mathbf{a}^* / \mathbf{b}^* / \mathbf{c}^*)$	(k_x, k_y, k_z)
$(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z}) = (k_x, k_y, k_z)\mathbf{P}$		
Reciprocal crystallographic primitive	$(\mathbf{a}^*_{\mathrm{P}} / \mathbf{b}^*_{\mathrm{P}} / \mathbf{c}^*_{\mathrm{P}})$	$(k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z})$
$(k_{\mathrm{ITA}x}, k_{\mathrm{ITA}y}, k_{\mathrm{ITA}z}) = (k_{\mathrm{P}x}, k_{\mathrm{P}y}, k_{\mathrm{P}z})\boldsymbol{Q}$		
Reciprocal “ITA description”	$(\mathbf{a}^*_{\mathrm{ITA}} / \mathbf{b}^*_{\mathrm{ITA}} / \mathbf{c}^*_{\mathrm{ITA}})$	$(k_{\mathrm{ITA}x}, k_{\mathrm{ITA}y}, k_{\mathrm{ITA}z})$
$(k_{\mathrm{R}x}, k_{\mathrm{R}y}, k_{\mathrm{R}z}) = (k_x, k_y, k_z)\mathbf{R}$		
Reciprocal “reduced” (triclinic only)	$(\mathbf{a}^*_{\mathrm{R}} / \mathbf{b}^*_{\mathrm{R}} / \mathbf{c}^*_{\mathrm{R}})$	$(k_{\mathrm{R}x}, k_{\mathrm{R}y}, k_{\mathrm{R}z})$

Fig. 1. Definition of reciprocal cells, transformation matrices between reciprocal cells, and symbols of reciprocal basis vectors and **k**-vector coefficients used in this study.

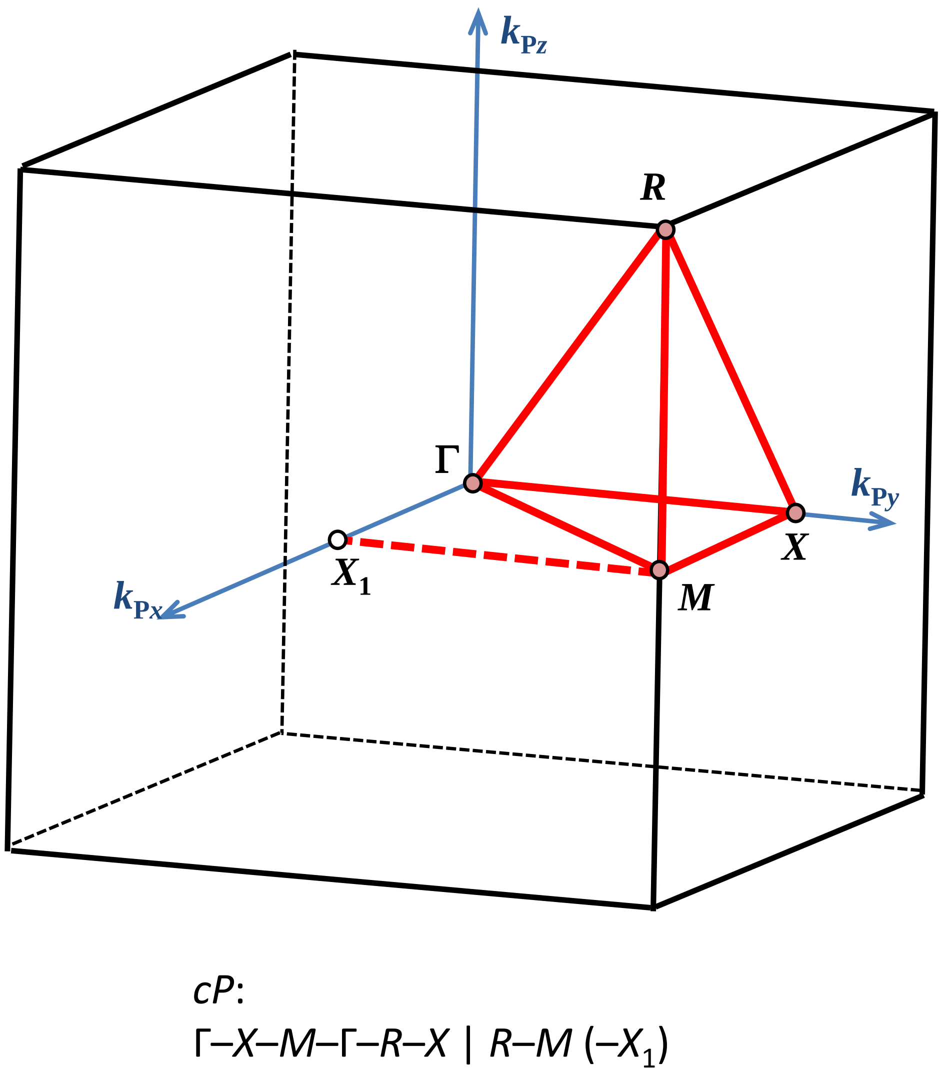
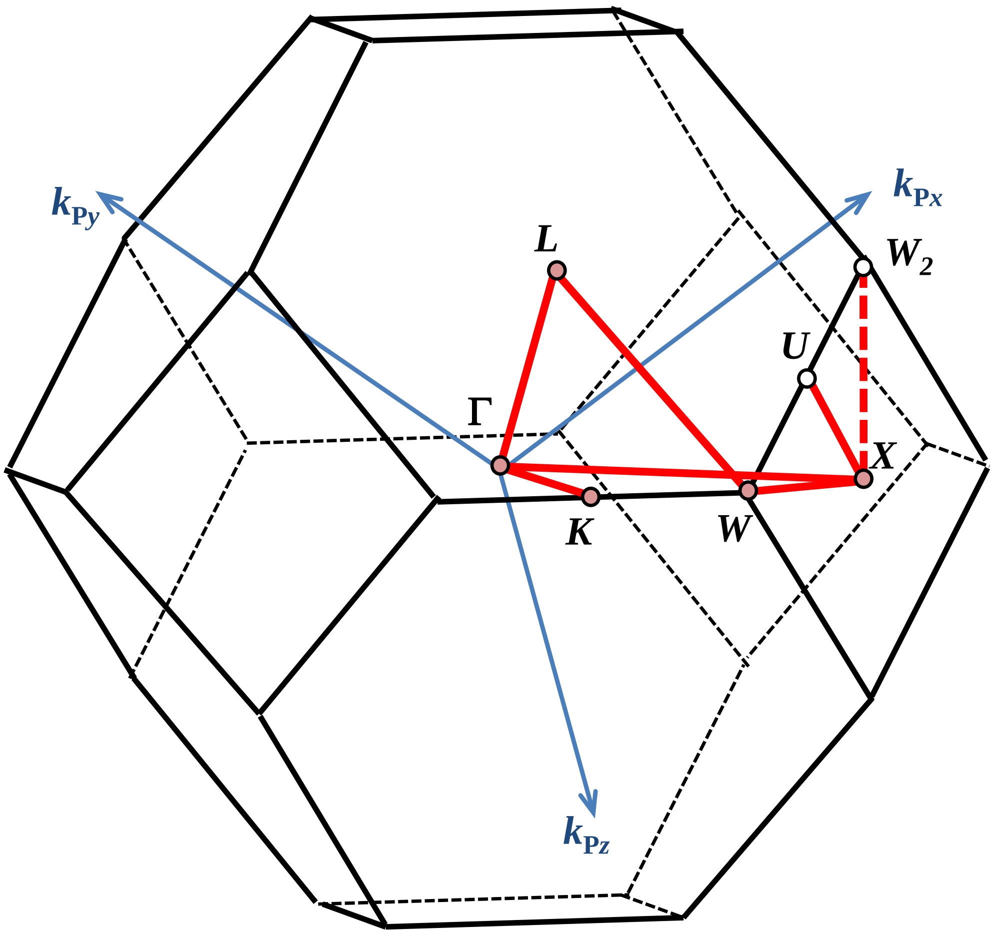


Fig. 2. The BZ, special BZ points, and recommended band path for *cP* lattices. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*X*–*M*–Γ–*R*–*X* | *R*–*M* (–X_1). The additional path *M*–X_1 is recommended for space group types $P23$, $P2_13$, $Pm\bar{3}$, $Pa\bar{3}$, and $Pn\bar{3}$ (numbers 195, 198, 200, 201, and 205, respectively).



cF:
Γ–X–U | K–Γ–L–W–X (–W_2)

Fig. 3. The BZ, special BZ points, and recommended band path for *cF* lattices. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–X–U | K–Γ–L–W–X (–W_2). The additional path X–W_2 is recommended for space group types $F23$, $Fm\bar{3}$, and $Fd\bar{3}$ (numbers 196, 202, and 203, respectively).

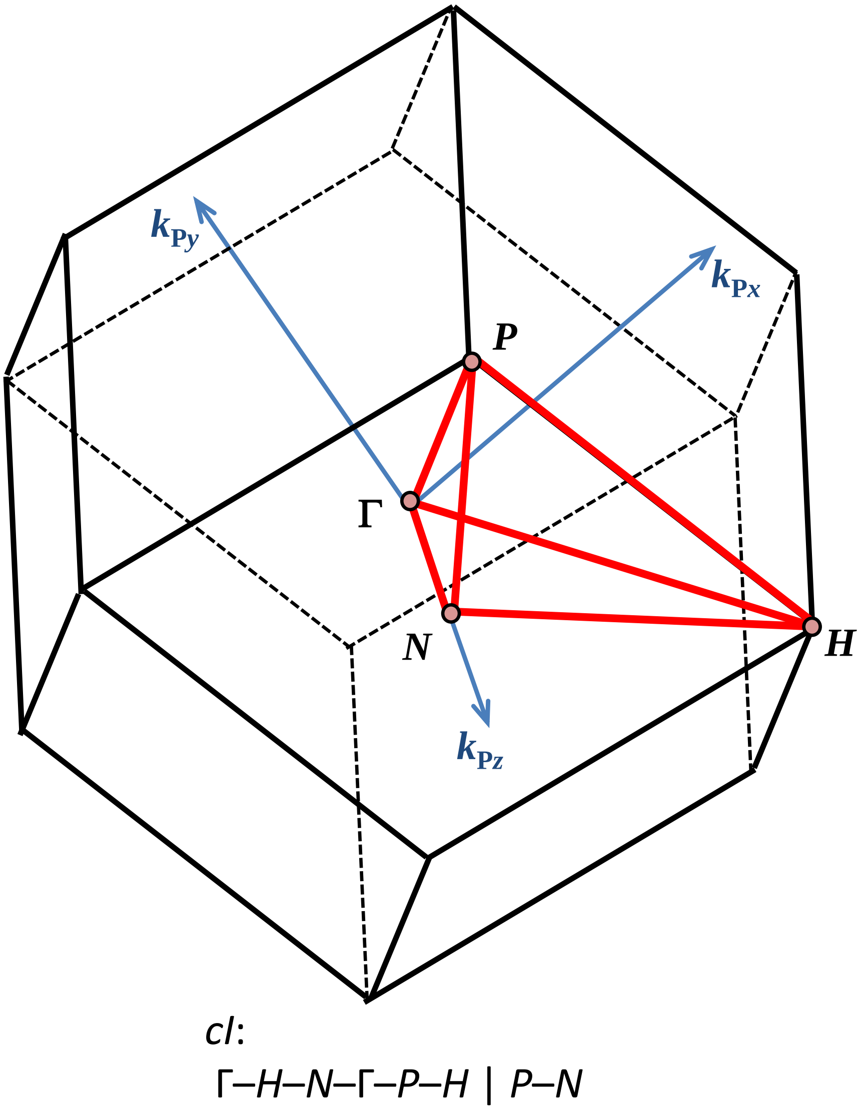
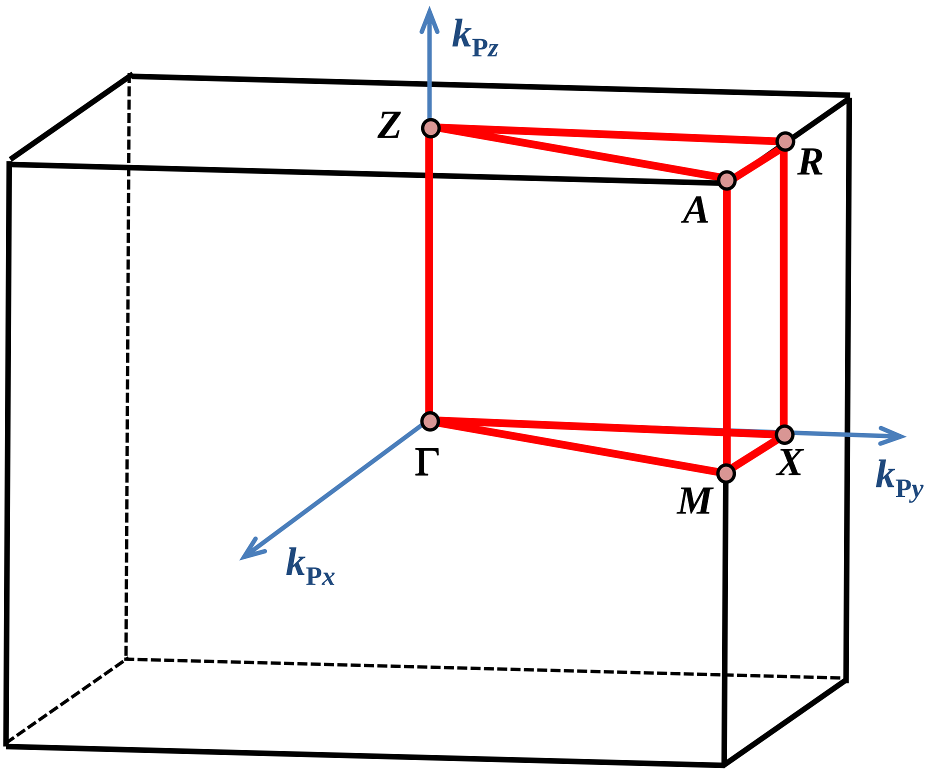


Fig. 4. The BZ, special BZ points, and recommended band path for *cI* lattices. Filled red circles indicate one representative of each special **k** -vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*H*–*N*–Γ–*P*–*H* | *P*–*N*.



tP:
Γ–*X*–*M*–Γ–*Z*–*R*–*A*–*Z* | *X*–*R* | *M*–*A*

Fig. 5. The BZ, special BZ points, and recommended band path for *tP* lattices. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*X*–*M*–Γ–*Z*–*R*–*A*–*Z* | *X*–*R* | *M*–*A*.

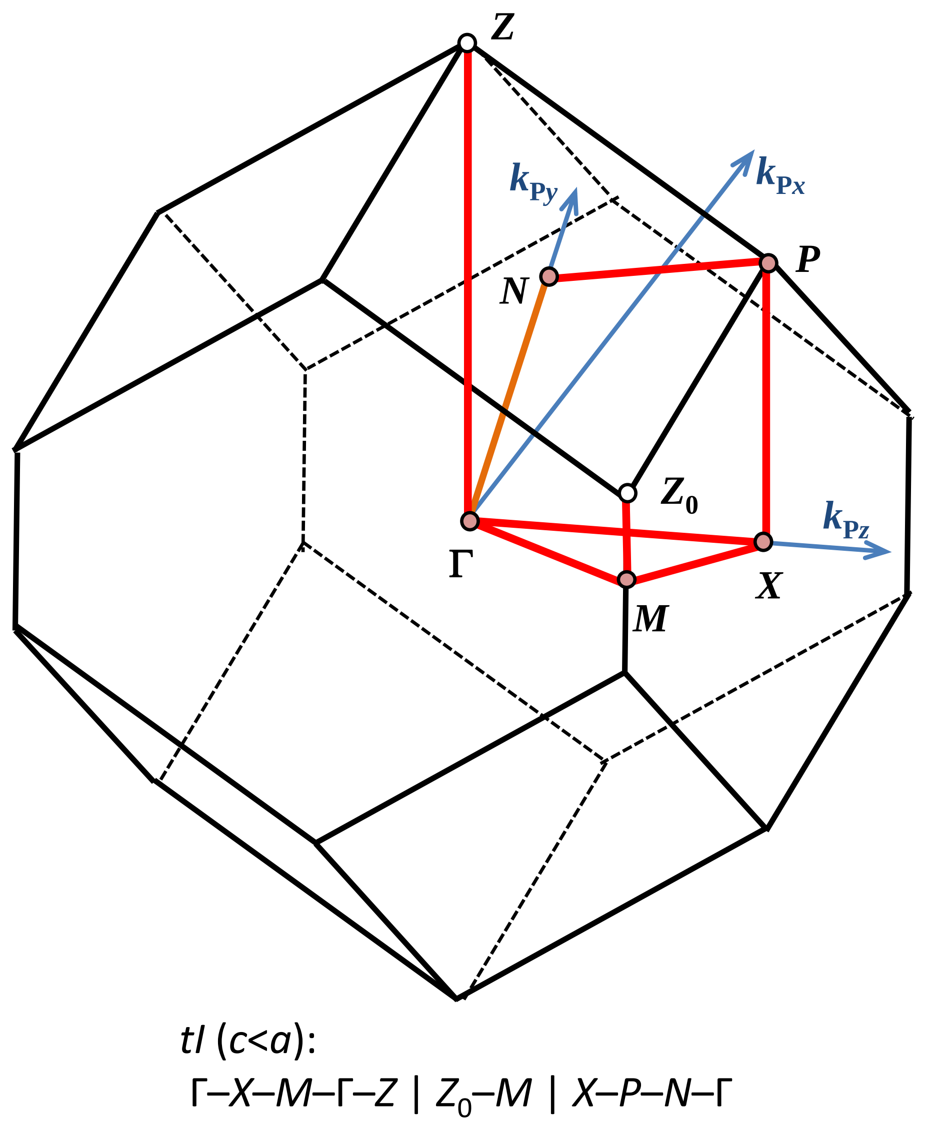


Fig. 6. The BZ, special BZ points, and recommended band path for *tI* lattices when $c < a$. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*X*–*M*–Γ–*Z* | Z_0–*M* | *X*–*P*–*N*–Γ.

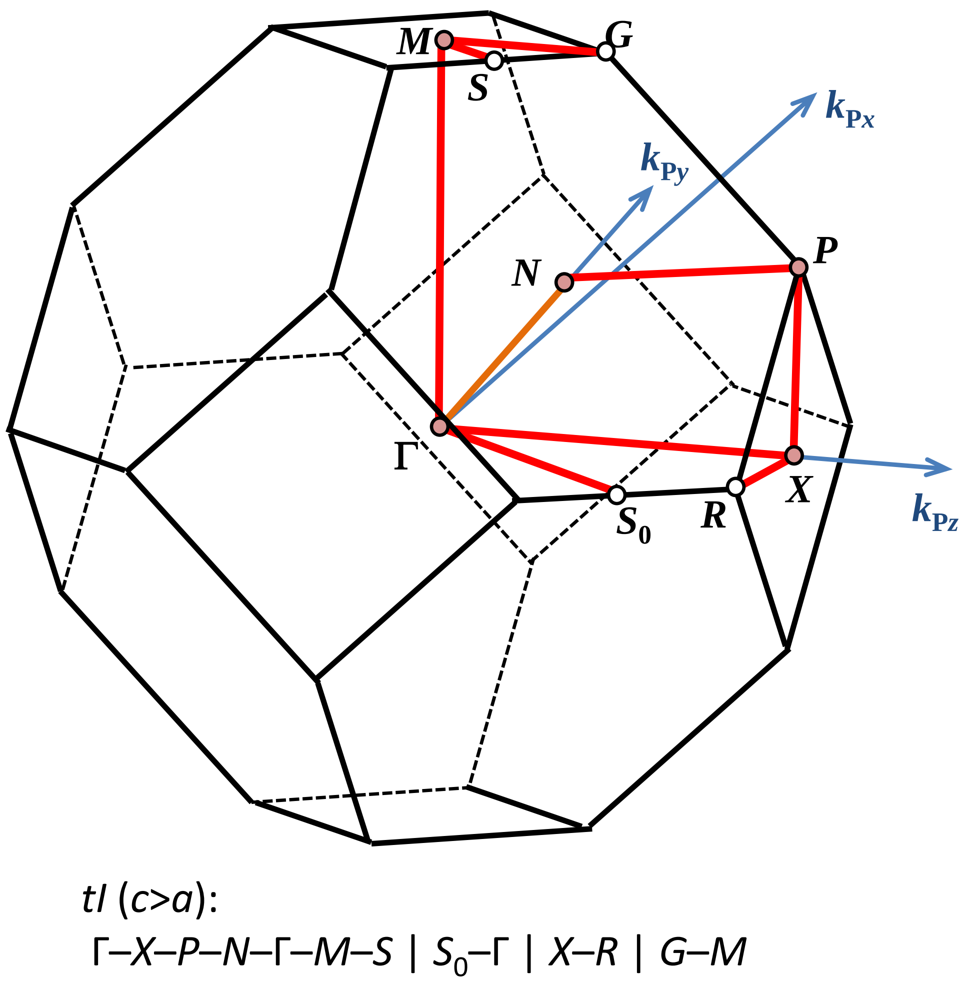
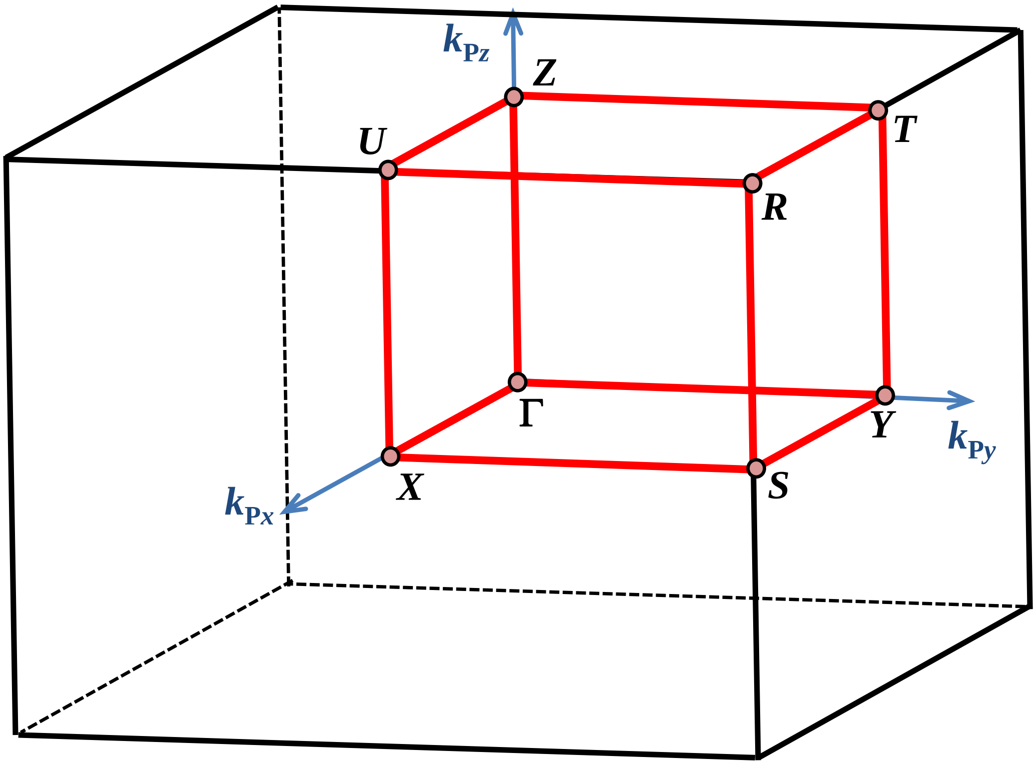


Fig. 7. The BZ, special BZ points, and recommended band path for *tI* lattices when $c > a$. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–X–P–N–Γ–M–S | S_0–Γ | X–R | G–M.



oP:
Γ–*X*–*S*–*Y*–Γ–*Z*–*U*–*R*–*T*–*Z* | *X*–*U* | *Y*–*T* | *S*–*R*

Fig. 8. The BZ, special BZ points, and recommended band path for *oP* lattices. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*X*–*S*–*Y*–Γ–*Z*–*U*–*R*–*T*–*Z* | *X*–*U* | *Y*–*T* | *S*–*R*.

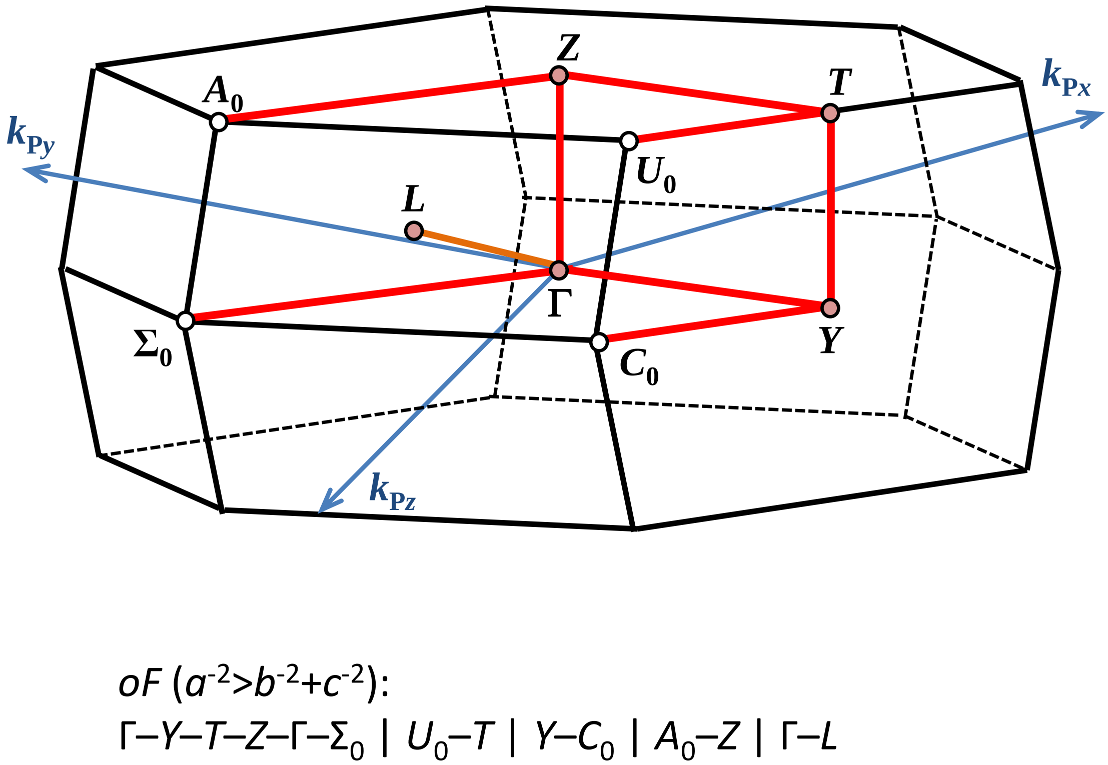
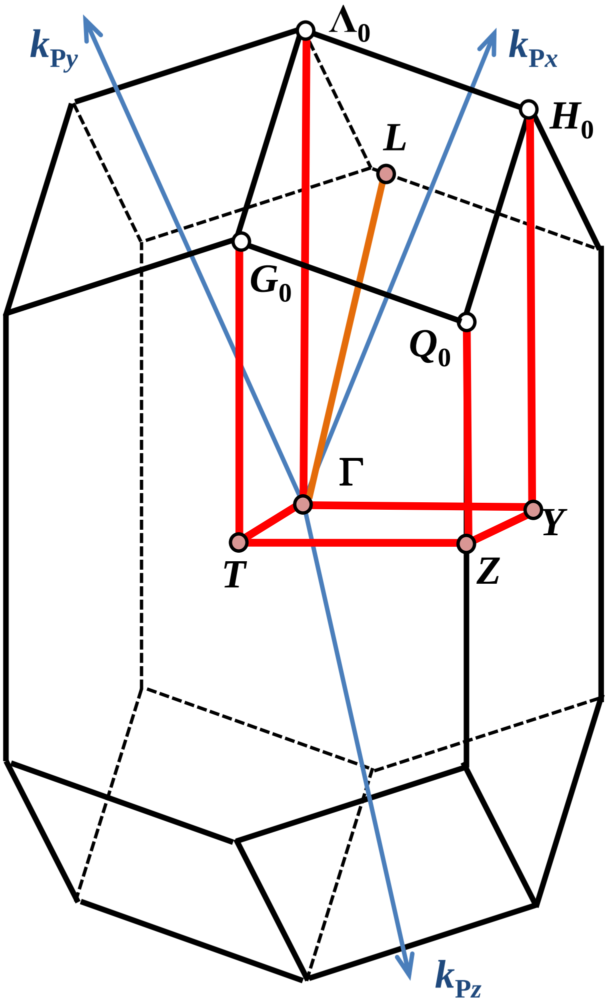


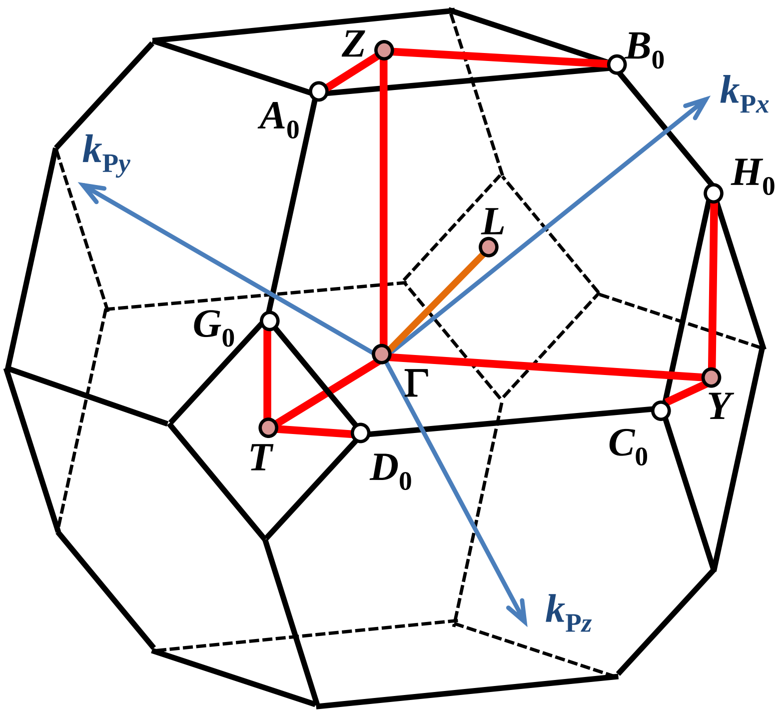
Fig. 9. The BZ, special BZ points, and recommended band path for *oF* lattices when $a^{-2} > b^{-2} + c^{-2}$. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–Y–T–Z–Γ–Σ_0 | U_0–T | Y–C_0 | A_0–Z | Γ–L.



oF ($c^{-2}>a^{-2}+b^{-2}$):

Γ–T–Z–Y–Γ–Λ_0 | Q_0–Z | T–G_0 | H_0–Y | Γ–L

Fig. 10. The BZ, special BZ points, and recommended band path for *oF* lattices when $c^{-2} > a^{-2} + b^{-2}$. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–T–Z–Y–Γ–Λ_0 | Q_0–Z | T–G_0 | H_0–Y | Γ–L.



oF (a^{-2}, b^{-2}, c^{-2} = edges of triangle):
Γ–Y–C_0 | A_0–Z–B_0 | D_0–T–G_0 | H_0–Y | T–Γ–Z | Γ–L

Fig. 11. The BZ, special BZ points, and recommended band path for *oF* when e a^{-2}, b^{-2}, and c^{-2} are edges of a triangle. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–Y–C_0 | A_0–Z–B_0 | D_0–T–G_0 | H_0–Y | T–Γ–Z | Γ–L.

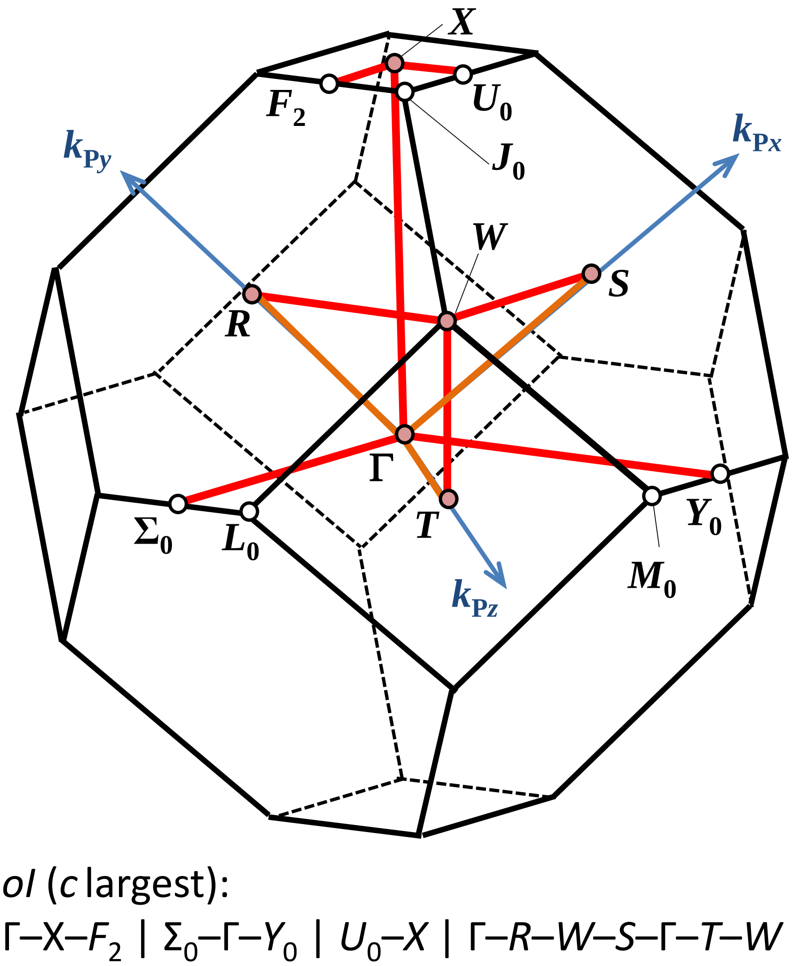


Fig. 12. The BZ, special BZ points, and recommended band path for oI when c is the largest. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–X–F_2 | Σ_0–Γ–Y_0 | U_0–X | Γ–R–W–S–Γ–T–W.

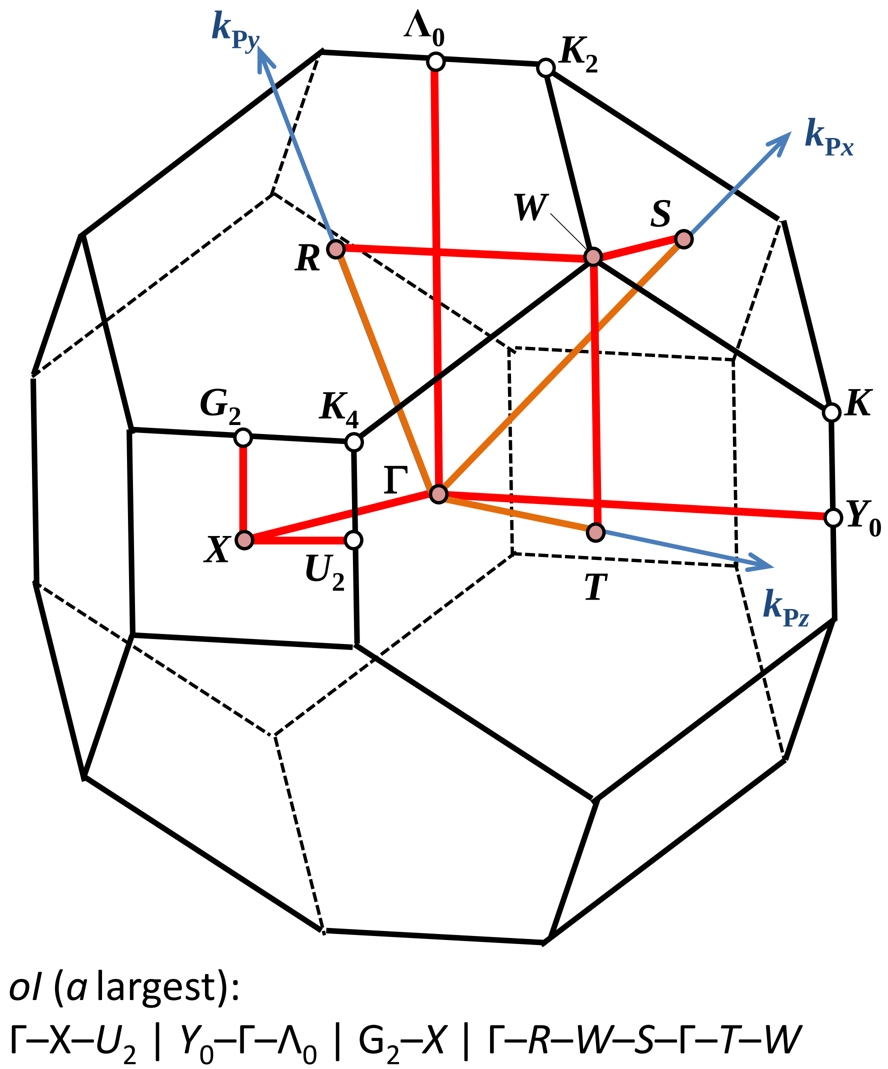
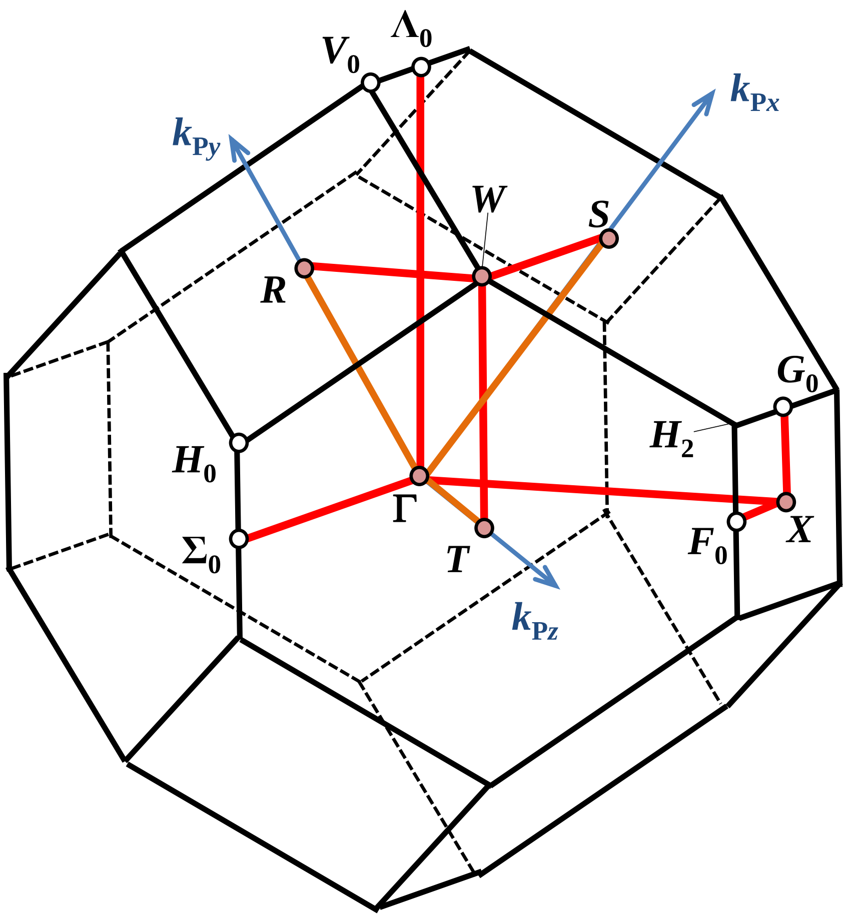


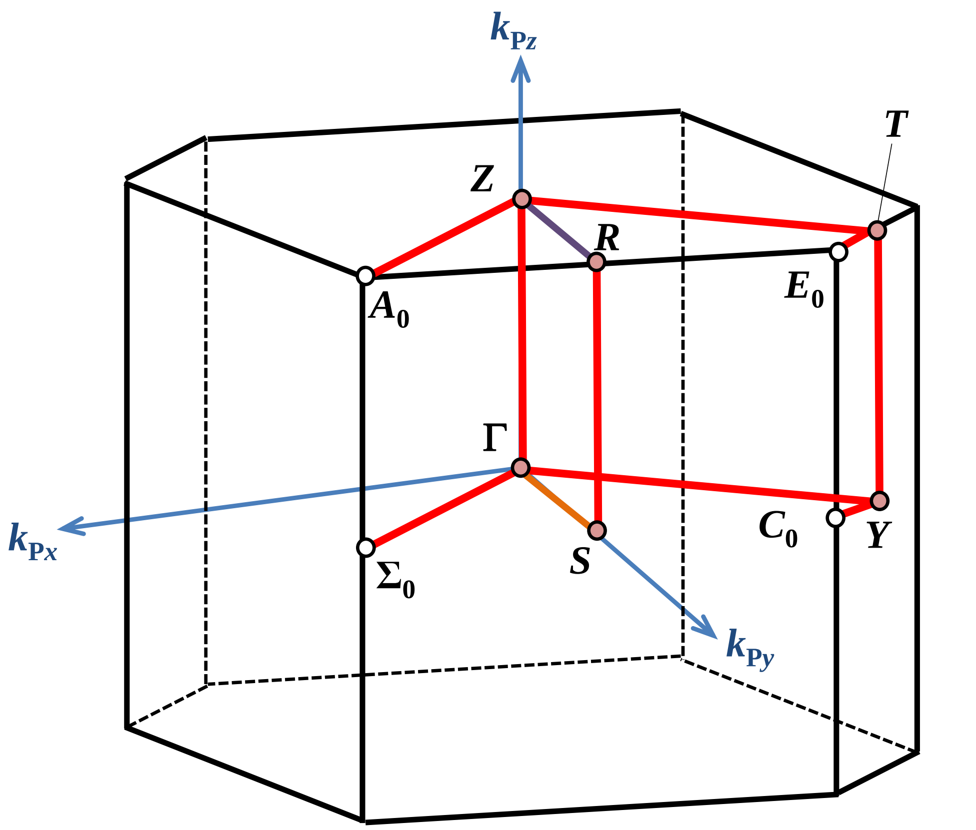
Fig. 13. The BZ, special BZ points, and recommended band path for *oI* when *a* is the largest. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–X–U_2 | Y_0–Γ–Λ_0 | G_2–X | Γ–R–W–S–Γ–T–W.



oI (*b* largest):

Γ–X–F_0 | Σ_0–Γ–Λ_0 | G_0–*X* | Γ–*R*–*W*–*S*–Γ–*T*–*W*

Fig. 14. The BZ, special BZ points, and recommended band path for *oI* when *b* is the largest. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–X–F_0 | Σ_0–Γ–Λ_0 | G_0–*X* | Γ–*R*–*W*–*S*–Γ–*T*–*W*.



oS (*a*<*b* if *oC*, *b*<*c* if *oA*):
Γ–*Y*–C_0 |Σ_0–Γ–*Z*–A_0 | E_0–*T*–*Y* | Γ–*S*–*R*–*Z*–*T*

Fig. 15. The BZ, special BZ points, and recommended band path for *oS* when $a < b$ if *oC* or $b < c$ if *oA*. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–Y–C_0 |Σ_0–Γ–Z–A_0 | E_0–T–Y | Γ–S–R–Z–T.

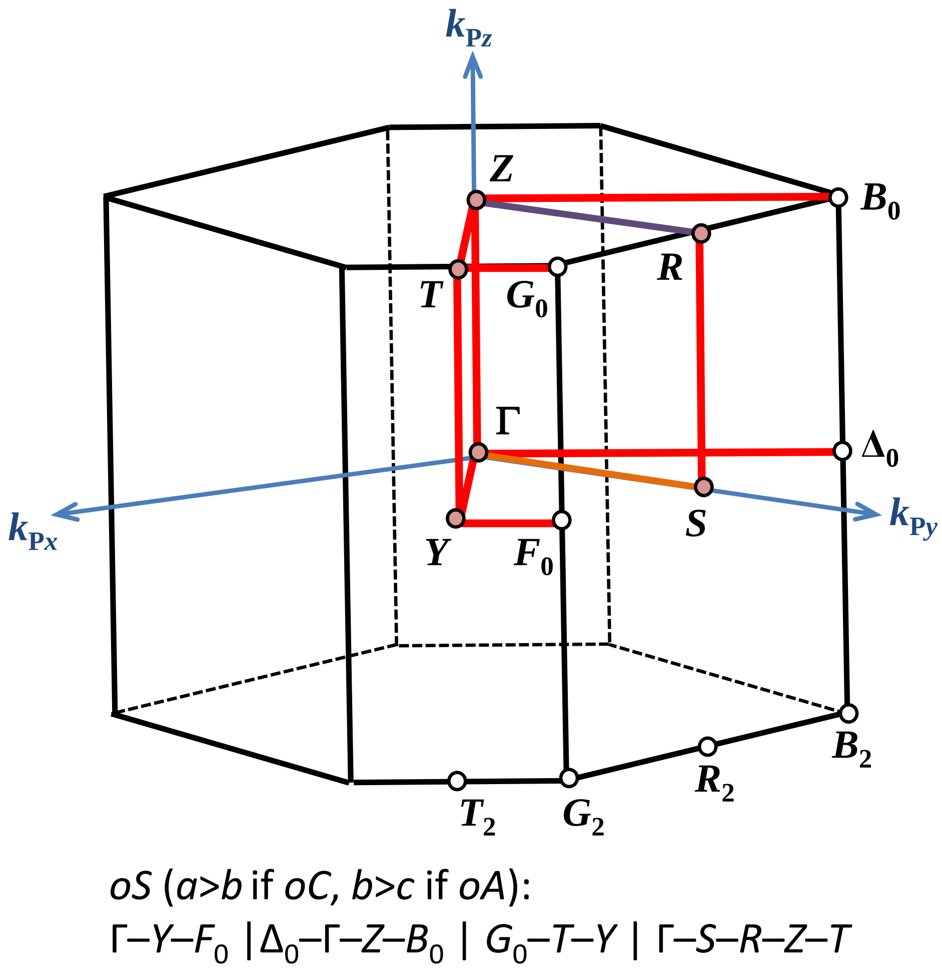
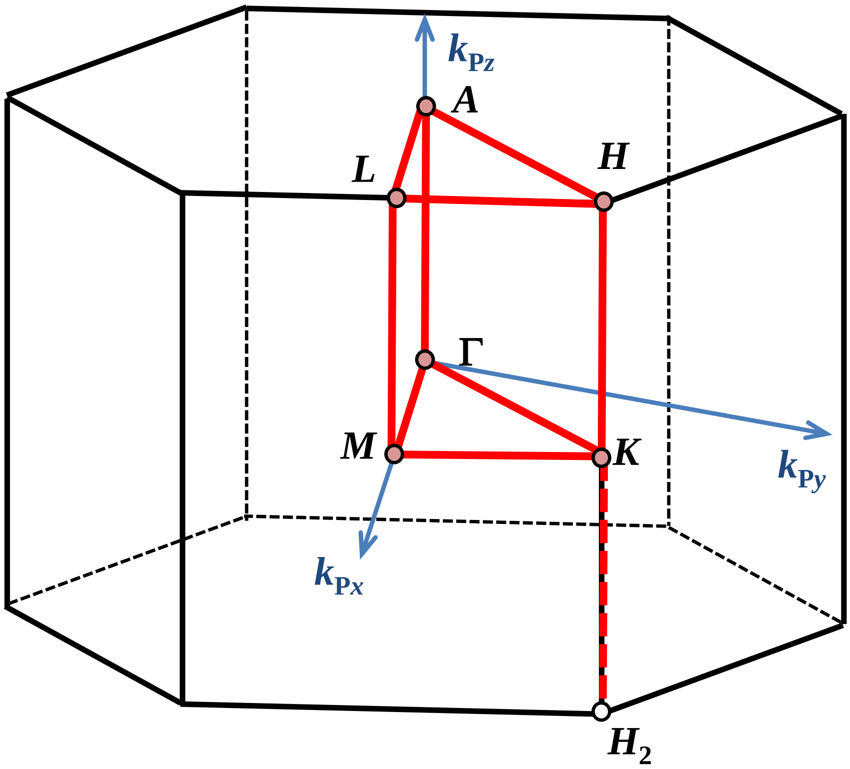


Fig. 16. The BZ, special BZ points, and recommended band path for *oS* when $a > b$ if *oC* or $b > c$ if *oA*. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–Y–F_0 | Δ_0–Γ–Z–B_0 | G_0–T–Y | Γ–S–R–Z–T.



hP:
Γ–*M*–*K*–Γ–*A*–*L*–*H*–*A* | *M*–*L* | *H*–*K*(–H_2)

Fig. 17. The BZ, special BZ points, and recommended band path for *hP*. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*M*–*K*–Γ–*A*–*L*–*H*–*A* | *M*–*L* | *H*–*K*(–H_2). The additional path *K*–H_2 is recommended for space group types *P*3, $P3_1$, $P3_2$, $P\bar{3}$, *P*312, $P3_112$ $P3_212$, *P*31*m*, P31*c*, $P\bar{3}1m$, and $P\bar{3}1c$ (numbers 143, 144, 145, 147, 149, 151, 153, 157, 159, 162, and 163, respectively).

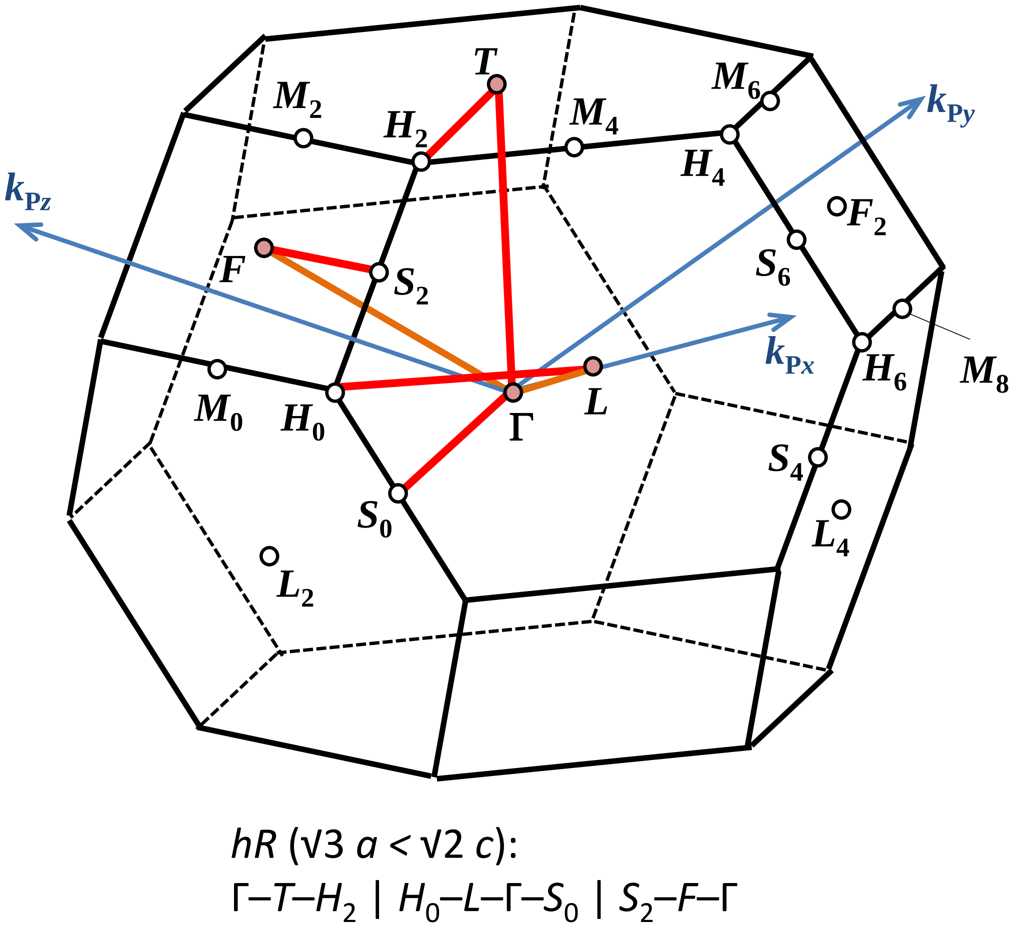
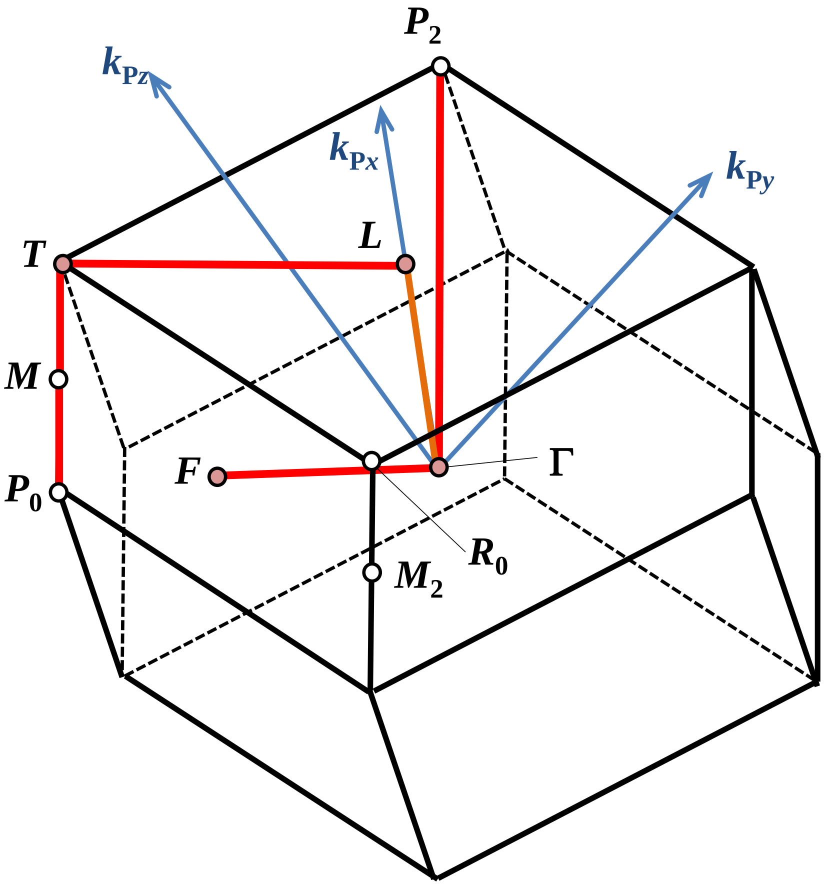
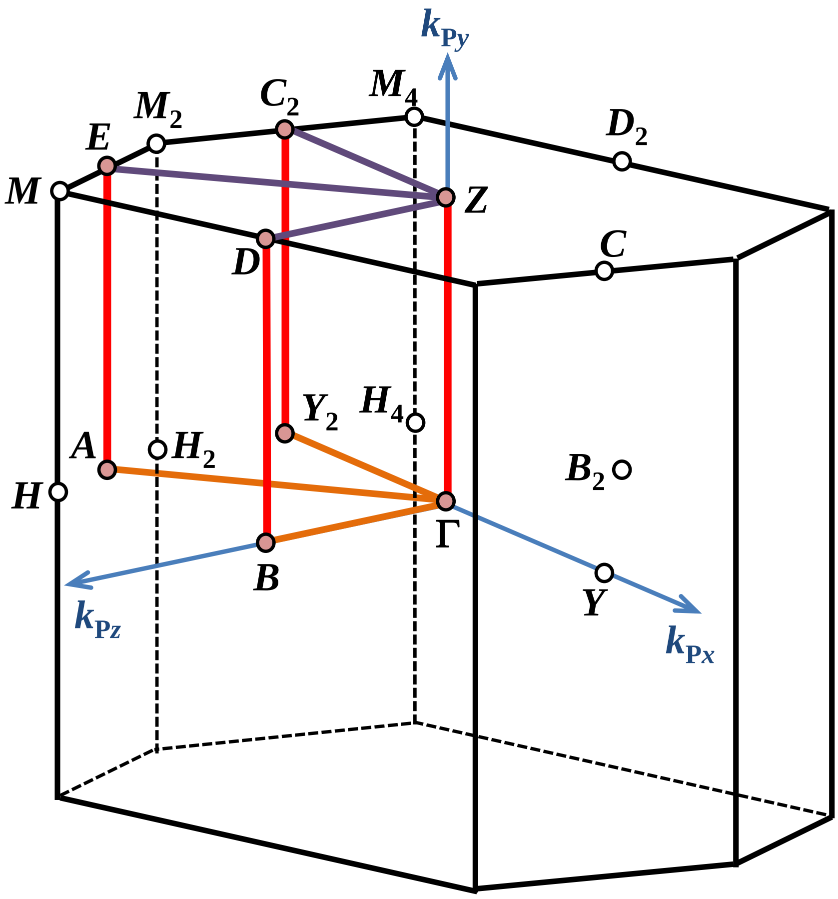


Fig. 18. The BZ, special BZ points, and recommended band path for *hR* when $\sqrt{3}a < \sqrt{2}c$. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–T–H_2 | H_0–L–Γ–S_0 | S_2–F–Γ.



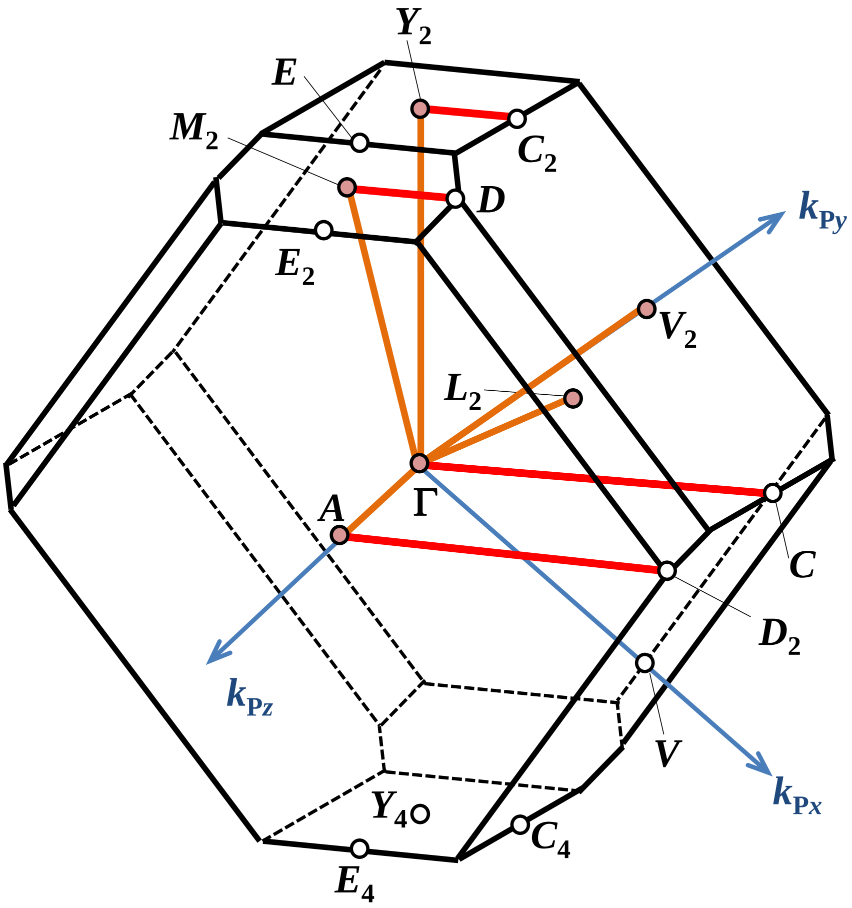
hR ($\sqrt{3}\,a > \sqrt{2}\,c$):
Γ–*L*–*T*–P_0 | P_2–Γ–*F*

Fig. 19. The BZ, special BZ points, and recommended band path for *hR* when $\sqrt{3}a > \sqrt{2}c$. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*L*–*T*–P_0 | P_2–Γ–*F*.



mP :
$\Gamma\text{–}Z\text{–}D\text{–}B\text{–}\Gamma\text{–}A\text{–}E\text{–}Z\text{–}C_2\text{–}Y_2\text{–}\Gamma$

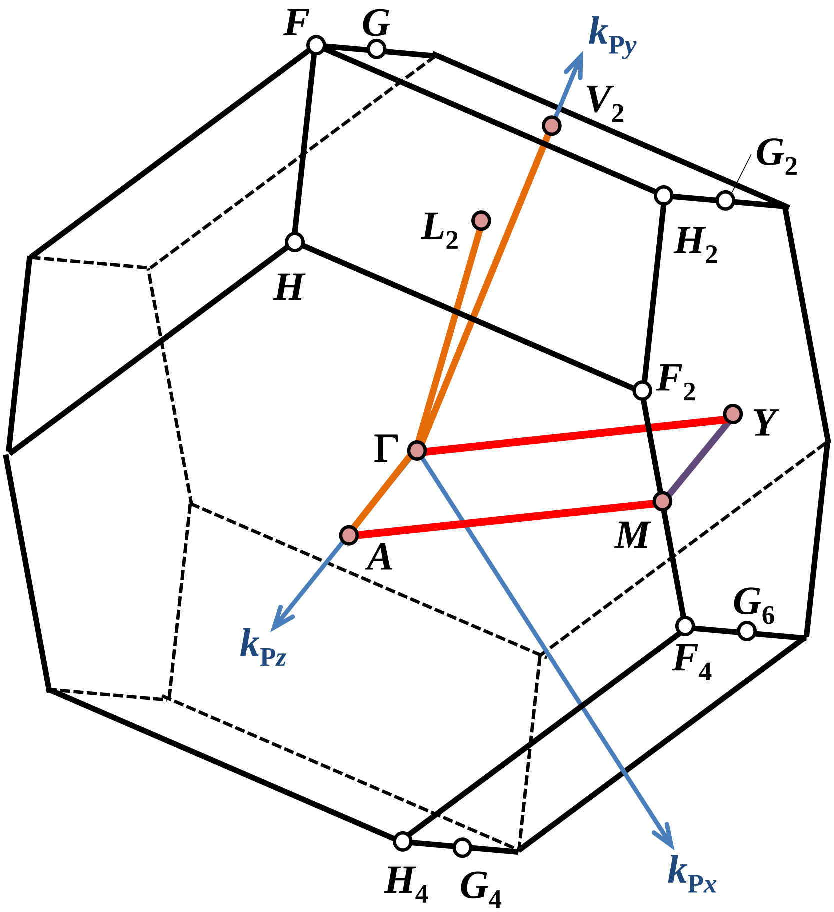
Fig. 20. The BZ, special BZ points, and recommended band path for *mP*. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is $\Gamma\text{–}Z\text{–}D\text{–}B\text{–}\Gamma\text{–}A\text{–}E\text{–}Z\text{–}C_2\text{–}Y_2\text{–}\Gamma$.



mC ($b<a\sin\beta$):

Γ–C | C_2–Y_2–Γ–M_2–D | D_2–A–Γ | L_2–Γ–V_2

Fig. 21. The BZ, special BZ points, and recommended band path for *mC* when $b < a\sin\beta$. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–C | C_2–Y_2–Γ–M_2–D | D_2–A–Γ | L_2–Γ–V_2.



mC (*b*>*a*sinβ elongated dodecahedron):
Γ–*Y*–*M*–*A*–Γ | L_2–Γ–V_2

Fig. 22. The BZ, special BZ points, and recommended band path for *mC* when $b > a\sin\beta$ and $-\dfrac{a\cos\beta}{c} + \dfrac{a^2\sin^2\beta}{b^2} < 1$. Filled red circles indicate one representative of each special $\mathbf{k}$-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*Y*–*M*–*A*–Γ | L_2–Γ–V_2.

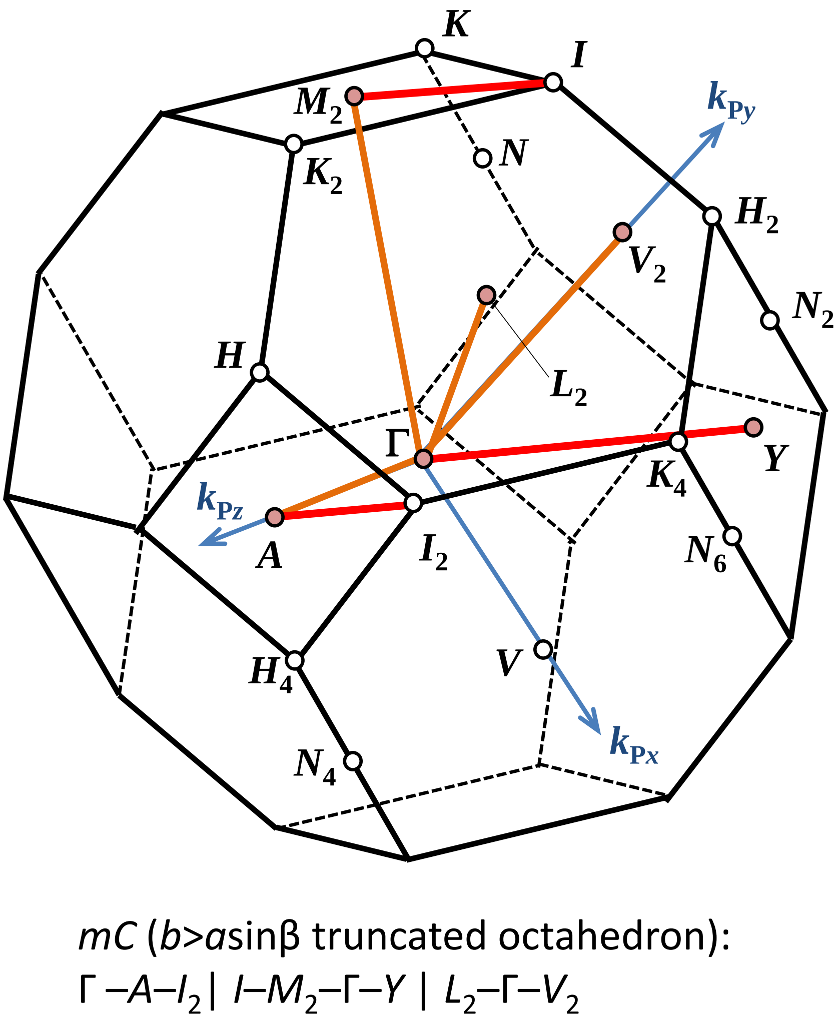
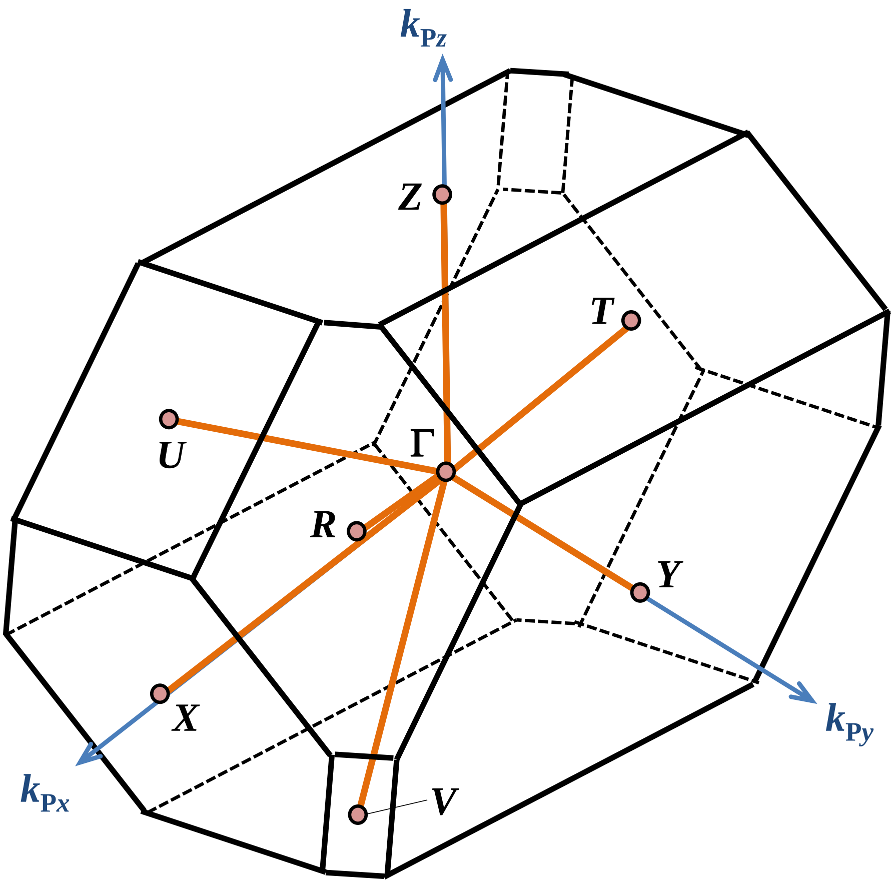
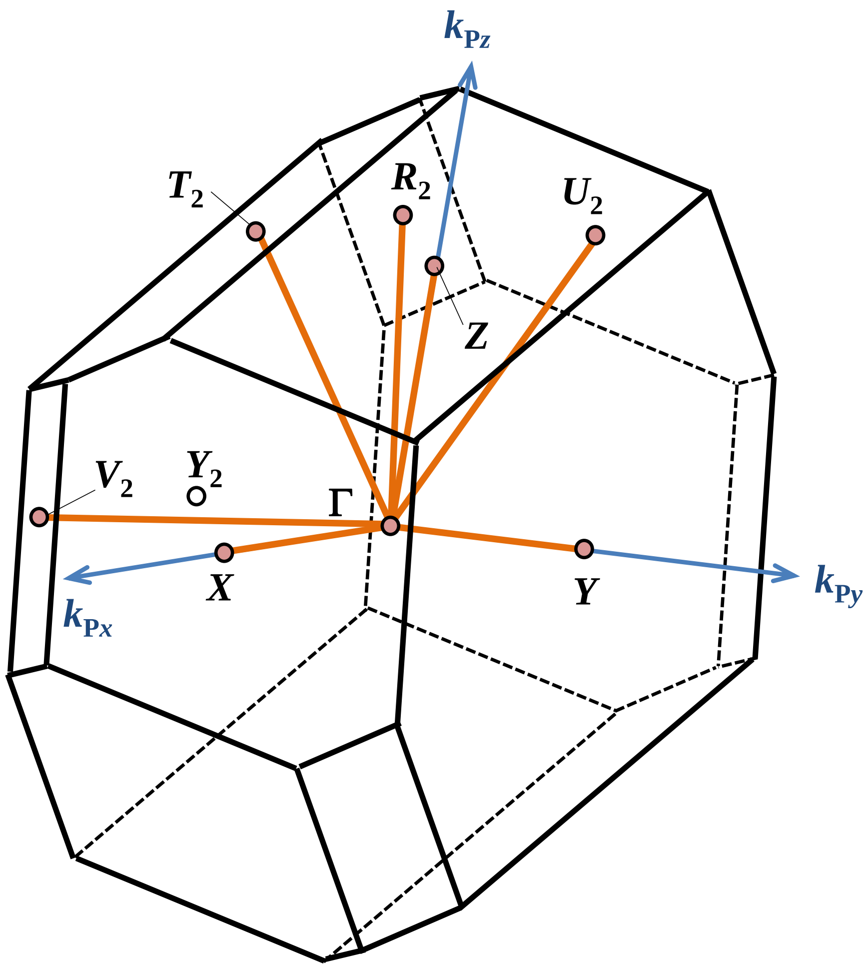


Fig. 23. The BZ, special BZ points, and recommended band path for *mC* when $b > a\sin\beta$ and $-\dfrac{a\cos\beta}{c} + \dfrac{a^2\sin^2\beta}{b^2} > 1$. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–A–I_2 | I–M_2–Γ–Y | L_2–Γ–V_2.



aP (reciprocal all-obtuse):
Γ–*X* | *Y*–Γ–*Z* | *R*–Γ–*T* | *U*–Γ–*V*

Fig. 24. The BZ, special BZ points, and recommended band path for *aP* when the interaxial angles of the reciprocal "reduced" cell are all-obtuse. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is Γ–*X* | *Y*–Γ–*Z* | *R*–Γ–*T* | *U*–Γ–*V*.



aP (reciprocal all-acute):
$\Gamma\text{–}X \mid Y\text{–}\Gamma\text{–}Z \mid R_2\text{–}\Gamma\text{–}T_2 \mid U_2\text{–}\Gamma\text{–}V_2$

Fig. 25. The BZ, special BZ points, and recommended band path for *aP* when the interaxial angles of the reciprocal "reduced" cell are all-acute. Filled red circles indicate one representative of each special **k**-vector point in the highest symmetry reciprocal space group type. The bold lines indicate segments of the recommended band path, which is $\Gamma\text{–}X \mid Y\text{–}\Gamma\text{–}Z \mid R_2\text{–}\Gamma\text{–}T_2 \mid U_2\text{–}\Gamma\text{–}V_2$.

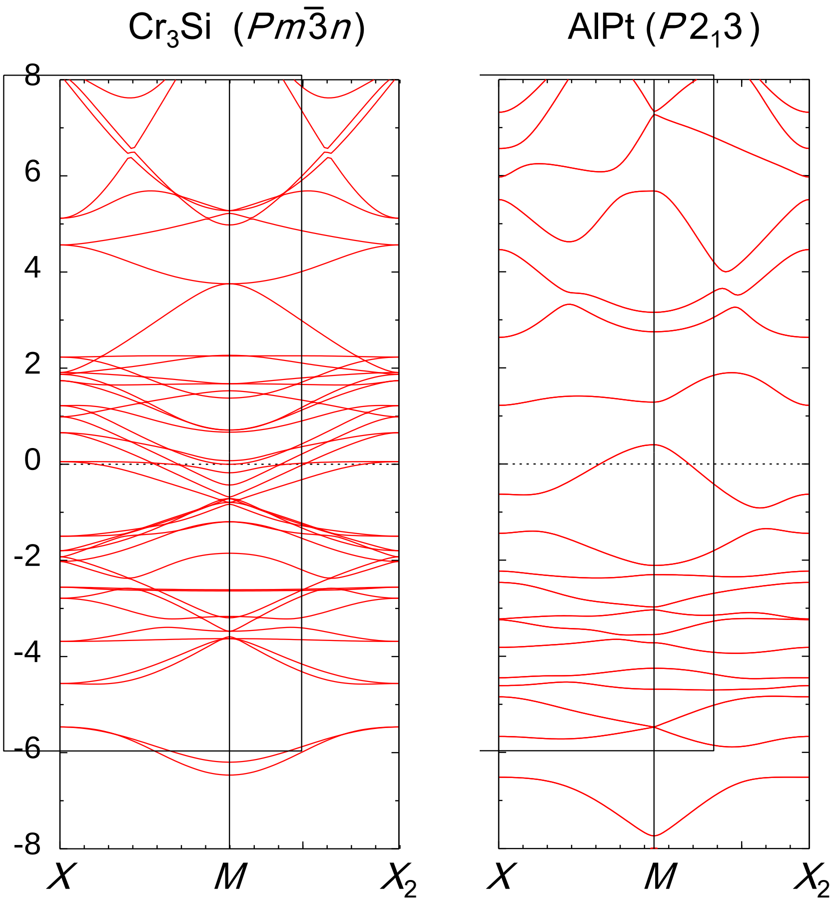


Fig. 26. Calculated band structure along band path X–M–X_2 for Cr_3Si and AlPt (space group types $Pm\bar{3}n$ and $P2_13$, numbers 223 and 198, respectively).