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Normally Supportive Sublattices of Crystallographic Space Groups

Miles A. Clemens

A thesis submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Master of Science

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ABSTRACT

Normally Supportive Sublattices of Crystallographic Space Groups

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Master of Science

Normal subgroups can be thought of as the primary building blocks for decomposing mathematical groups into quotient groups. The properties of the resulting quotient groups are often used to determine properties of the group itself. This thesis considers normal subgroups of three-dimensional crystallographic space groups that are themselves three-dimensional crystallographic space groups; for convenience, we refer to such a subgroup as a csg-normal subgroup. We identify practical restrictions on csg-normal subgroups that facilitate their tabulation. First, the point group of an csg-normal subgroup must be a normal subgroup of the crystallographic point group of the space group, which we refer to for convenience as a cpg-normal subgroup. For each of the cpg-normal subgroups, which are all well known, we identify the abstract quotient group. Secondly, we identify necessary conditions on the sublattice basis of any csg-normal subgroup, and tabulate the "normally supportive" sublattices that meet these conditions, where some tables are symbolic forms that represent infinite families of sublattices. For a given space group, every csg-normal subgroup must be an extension of such a normally supportive sublattice, though some normally supportive sublattices may not actually support such extensions.

Keywords: space groups, normal subgroups, crystallography

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Contents

Table of Contents	iv
List of Figures	vi
1 Introduction	1
1.1 Groups and Crystal-Symmetry Groups	1
1.2 A Simple Example	3
1.3 Affine Matrix Representation of Space-Group Elements	4
1.4 Applications of Normal Subgroups of Space Groups	5
1.5 Goals and Strategy	6
1.6 Motivating Example: Domain Structure of YMnO_3	7
2 Point Groups	11
2.1 Normal Subgroups and Quotients of Crystallographic Point Groups	11
3 Normally Supportive Sublattices	15
3.1 The Hermite Normal Form of a Sublattice Basis	15
3.2 Normally Supportive Conditions	16
3.3 Inclusion Sublattices	18
3.4 The Extension Problem	24
4 Algorithm	26
4.1 Overview	26
4.2 Subroutines	27
5 Results and Discussion	32
5.1 Tables	32
5.2 Validation	38
6 Examples	40
6.1 A Simple Case	40
6.2 A Case with Bifurcation	43
6.3 A Case with Extra Conditions	45

6.4 A Very Messy Case	48
7 Conclusions and Future Work	55
Bibliography	58
Appendix A Normally Supportive Sublattices	62

List of Figures

1.1	Dihedral Group	3
1.2	Commutative Diagram	7
1.3	Unit Cells of YMnO ₃ Domains	8
1.4	Topological Defect in YMnO ₃	9
1.5	Coset Graph of YMnO ₃ Domains	10

List of Tables

2.1	Normal Subgroups and Quotients of Point Groups	13
2.2	Abstract Groups	14
3.1	Inclusions	19
5.1	Overview of Normally Supportive Sublattices	33
A.1	Normally Supportive Sublattices	62
A.2	Extra Conditions	128

Chapter 1

Introduction

1.1 Groups and Crystal-Symmetry Groups

A group, by definition, is a set with a binary operation with the following four properties: closure, associativity, an identity, and inverses for each element [1–4]. Closure means that the product of any two elements in the group will result in another element in the group (it is common to refer to the binary operation as multiplication and the result as the product). Associativity means that the order of operations is irrelevant, that is $a(bc) = (ab)c$ for any elements a , b , and c in the group. The identity is an element (usually denoted as e) that leaves any other element invariant, that is to say $ae = a$ for any element a in the group. The inverse of an element (usually denoted by -1 in the superscript) is the element that returns the identity when multiplied by the original element, that is to say $a^{-1}a = e$ for any element a in the group.

We say that two elements $a, b \in G$ are conjugate elements if there exists some $g \in G$ such that $a = g^{-1}bg$. Any set of elements in G that are all mutually conjugate is known as a conjugacy class. The set of all conjugacy classes of elements in G partition the group, meaning that they are mutually disjoint and that their union is G . The identity is always alone in a conjugacy class since

$g^{-1}eg = g^{-1}g = e$ for every $g \in G$.

A subgroup H of G is a subset of G that possesses all of the properties that define a group under the same binary operation [1–4]. If H is a subgroup of G , which we denote as $H \subseteq G$, then for any $a \in G$ we call the set $aH = \{ah|h \in H\}$ a coset of H in G containing a . If $N \subseteq G$ such that $aN = Na$ for every element $a \in G$ then we call N a normal subgroup of G , which we denote as $N \trianglelefteq G$ [1, 2, 4]. A normal subgroup will only contain complete conjugacy classes of the parent, or in other words, either all of the elements in a conjugacy class are in the normal subgroup or none of them are. If $H \subseteq G$, then we call the largest subgroup of H that is normal in G the normal core of H in G , and denote it as $N_H(G)$.

A normal subgroup $N \trianglelefteq G$ is special in that the set of its cosets in G form a group under the coset multiplication operation: $(aN)(bN) = abN$ for any $a, b \in G$ (subgroups that are not normal do not have this property). This group of cosets is known as a quotient group (sometimes called a factor group) and is denoted by G/N [1–4]. Coset multiplication is not well defined for a non-normal subgroup.

Group theory is relevant to the study of crystalline structures because the symmetries of a crystal form a group. A symmetry is any action on an object that leaves the object invariant. More generally, the symmetries of any physical system (e.g. an object, field, collection of objects and fields, model, or physical theory) form a group, wherein the group elements are transformations of the system and where the binary operation is composition. For objects like molecules and crystals, the relevant symmetries are geometric Euclidean isometries, which can be translations, point operations, or combinations of the two. A point symmetry leaves at least one point invariant. Examples are inversion, reflection about a plane, or rotation around a line. A translation symmetry translates the entire space by a fixed vector amount. The set of all point symmetries possessed by a crystal comprise a crystallographic point group [3]. The set of all symmetries possessed by a crystal comprise a crystallographic space group. A space group contains point symmetries,

translational symmetries, and combinations of the two (glide planes and screw axes) [1, 3]. The set of all pure translational symmetries possessed by a crystal comprise a crystallographic lattice group. This infinite lattice, whose rank is the dimension of the crystal, is a normal subgroup of the space group of the crystal. We will only consider three-dimensional crystals in the present work.

1.2 A Simple Example

To illustrate the concepts presented above, consider the six point symmetries of a 2D equilateral triangle, which form the dihedral group denoted as D_3 . Let us define the composition ab of geometric symmetries a and b such that the action of b is applied to the object first, followed by the action of a .

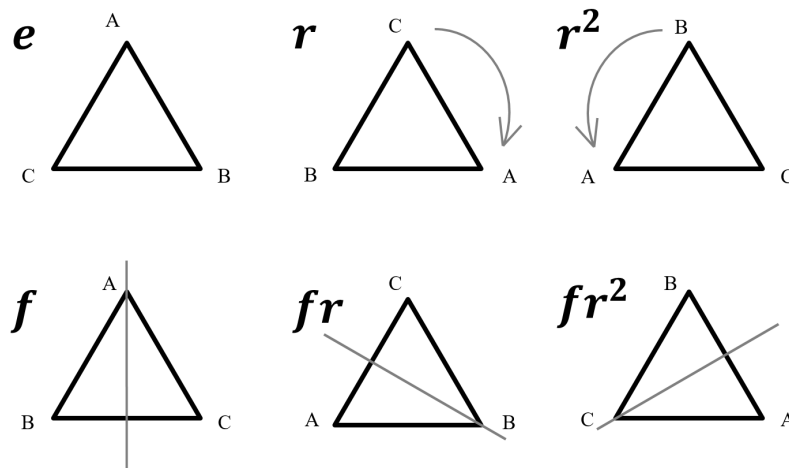


Figure 1.1 The symmetries of an equilateral triangle, commonly known as the dihedral group of order 6 and denoted as D_3 .

The subgroups of D_3 are $\{e\}$, $\{e, f\}$, $\{e, fr\}$, $\{e, fr^2\}$, $\{e, r, r^2\}$, and $\{e, r, r^2, f, fr, fr^2\}$. Of these subgroups, both $\{e\}$ and D_3 are obviously normal subgroups. If we let $H = \{e, r, r^2\}$ then H has two possible cosets, namely $eH = rH = r^2H = \{e, r, r^2\}$ and $fH = frH = fr^2H = \{f, fr, fr^2\}$. Furthermore, we can see that $He = Hr = Hr^2 = \{e, r, r^2\}$ and $Hf = Hfr = Hfr^2 = \{f, fr, fr^2\}$.

Thus for any element $a \in D_3$, $aH = Ha$ so that $\{e, r, r^2\}$ is a normal subgroup of D_3 . If we instead choose $H = \{e, fr\}$, the cosets of H are $eH = frH = \{e, fr\}$, $rH = fH = \{r, f\}$, and $r^2H = fr^2H = \{r^2, fr^2\}$. However, $Hr = \{r, fr^2\} \neq rH$ so that $\{e, fr\}$ is not a normal subgroup of D_3 . We see that $\{e\}$, $\{e, r, r^2\}$, and D_3 are the only normal subgroups of D_3 .

The cosets of the normal subgroup $N = \{e, r, r^2\}$ are $N = \{e, r, r^2\}$ and $fN = \{f, fr, fr^2\}$. Under coset multiplication, $(N)(N) = (fN)(fN) = \{e, r, r^2\} = N$ and $(N)(fN) = (fN)(N) = \{f, fr, fr^2\} = fN$. Thus with N as the identity, $\{N, fN\}$ is a group under the coset multiplication operation. In contrast, the cosets of non-normal subgroup $H = \{e, fr\}$ are $H = \{e, fr\}$, $rH = \{r, f\}$, and $r^2H = \{r^2, fr^2\}$, in which case $(rH)(r^2H) = \{e, r^2, fr, fr^2\}$ which is not one of the cosets of H . Because the cosets do not satisfy the closure condition, they do not form a group.

1.3 Affine Matrix Representation of Space-Group Elements

We find it convenient to use 4×4 affine-transformation matrices to represent the elements of a crystallographic space group, which allows us to employ matrix multiplication in performing symmetry-group calculations. The matrices are defined in the usual way relative to a basis of the lattice group of the crystal.

As an example, let g be a 2_1 screw axis in the $+z$ direction. The affine matrix representation of g is

$$g = \begin{pmatrix} p_g & t_g \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (1.1)$$

where p_g is a 3×3 matrix representing the point symmetry part and t_g is a 3×1 translation vector.

Every affine matrix has a 1×3 block of zeros on the bottom row followed by a 1 in the bottom right corner.

The application of this affine matrix is the equivalent of applying the point operation first and then the translation. For example, the action of g on coordinate $\chi = (x, y, z)$ is

$$g\chi = p_g \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t_g = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ z + \frac{1}{2} \end{pmatrix}. \quad (1.2)$$

In other words, it will map the coordinate (x, y, z) to $(-x, -y, z + \frac{1}{2})$.

The International Tables for Crystallography presents representative space group elements (one for each coset of the translation subgroup) of each space group in terms of their action on coordinate (x, y, z) . The conversion of this action into affine matrix form is very straightforward.

1.4 Applications of Normal Subgroups of Space Groups

Normal subgroups and the corresponding quotients have seen a number of important applications in the context of crystallography. Let $H \subseteq G$ and let K be the smallest subgroup of G such that H is a proper normal subgroup of K ; K is then known as the normalizer of H in G [5]. Normalizers (Euclidean or affine) are commonly used for the identification of equivalent but symmetrically-unrelated Wyckoff orbits or crystal-structure coordinate descriptions [6–8]. The subperiodic groups (e.g. layer, rod, and frieze groups) of space groups have been systematically classified via their isomorphisms to space-group quotients [9, 10]. Quotient groups of space groups with respect to normal subgroups are also employed in the construction of symmetry groups in higher than three dimensions via the use of subdirect products [11–13]. Subperiodic groups are associated via scanning tables with the symmetries of interfaces between crystal domains below a phase transition [14, 15]. For a low-temperature phase transition giving rise to a ferroelectric space group (or ferromagnetic space group) H relative to a paraelectric (or paramagnetic) parent space-group G , the ferroic domains correspond to the cosets of H in G , and the action of the normal core

$N_H(G)$ on these cosets reveals the minimal symmetry of a multi-domain crystal with a spatially balanced domain configuration [16–18]. The ISOTROPY software program employs the action of the normal core to identify symmetry-unique domain-pair interfaces [19].

In 1987, Kopský laid out plans to identify and understand the normal subgroups of crystallographic space groups, and expected to follow his first article on this topic with a series of more specific results, though the subsequent articles never came to fruition. In that same article, he showed that only space groups that are irreducible (there is not a subgroup of the translation group that is left invariant the point group) have a finite number of csg-normal subgroups with nontrivial point groups [20]. A year later, it was reported that a table of normal subgroups of reducible space groups "require too much volume to be published in a journal" [21], which is a slightly odd statement given that the number of normal subgroups in such a case is actually infinite. In any case, the difficulty of the situation was clearly recognized. The present work is a key step towards an exhaustive table of three-dimensional normal subgroups of three-dimensional crystallographic space groups. One of our essential innovations has been the preparation of a finite table of infinite families of normally supportive sublattices in symbolic matrix form. Though Kopský and others clearly envisioned progress in this area, the computational tools that we used for symbolic algebraic reduction and manipulation were not available at that time.

1.5 Goals and Strategy

In the future, we hope to classify all csg-normal subgroups of each of the 230 crystallographic space groups, as well as the corresponding quotient groups. To accomplish this, our strategy is outlined as follows. Firstly, a space group G is broken down into its point group, P_G , and its translation group, T_G . Secondly, all the normal subgroups of the point groups, $P_N \trianglelefteq P_G$, are found individually. Thirdly, for each P_N , we must find the normal subgroups of the translation group,

$T_N \trianglelefteq T_G$, that support the normality of $T_N \rtimes P_N$ in G (the symbol \rtimes indicates a semidirect product); we explain what it means to support normality below in chapter 3 [12, 22]. Fourthly, identify extensions N of P_N by T_N such that $N \trianglelefteq G$ (i.e. non-symmorphic space groups in the arithmetic crystal class of symmorphic space group $T_N \rtimes P_N$).

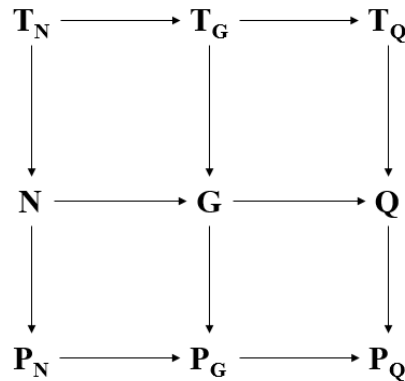


Figure 1.2 A commutative diagram consisting of short, exact sequences. The first arrow in any straight line points to a group from a normal subgroup of that group (e.g. $N \trianglelefteq G$). The second arrow points to the quotient of the two groups (e.g. $Q = G/N$).

1.6 Motivating Example: Domain Structure of $YMnO_3$

Here, we provide a motivating example that illustrates the use of csg-normal subgroups of a space group. Consider the domains of hexagonal yttrium manganite ($YMnO_3$). $YMnO_3$ has a symmetry-lowering ferroelectric phase transition at 1258K wherein atoms are displaced along the hexagonal c axis to form a low-symmetry hexagonal phase [23]. Below the transition temperature, there are six possible domains of the low temperature child structure which correspond to different directions of the ferroelectric and antiferroelectric order parameters [24]. The ferroelectric order parameter displaces all atoms of a given type in the same direction, whereas the antiferroelectric order parameter displaces some atoms of a given type in the $+z$ direction and the others in the $-z$ direction (see Figure 1.3) [25]. These six domains have been observed to meet at a one-dimensional

topological defect, around which they form a six-fold pinwheel pattern (see Figure 1.4) [26,27].

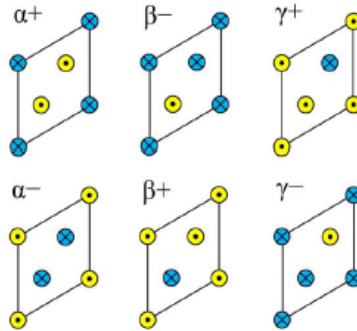


Figure 1.3 The displacements of yttrium atoms in the unit cells of each $YMnO_3$ domain. [25]

Here, the space group H of the low temperature phase ($P6_3cm$, #185) is a subgroup of the space group G of the high temperature phase ($P6_3/mmc$, #194); or in other words, $H \subseteq G$ [23]. However, because $H \not\trianglelefteq G$, the cosets of H in G do not form a quotient group, though the cosets of the normal core, $N_H(G)$ ($P3c$, #158), do result in a quotient group $Q = G/N_H(G)$. Because Q is a group of cosets of H in G , every element of G acting on a coset is guaranteed to return another coset by closure. In other words, the action of G permutes the elements of Q . This is physically meaningful because there is a one to one correspondence between the cosets of H in G and the physical domains of the $YMnO_3$ crystal [28]. The elements of G permute the elements of Q in the same way the symmetries of the parent space group permute the low-temperature domains.

To visualize the physical significance of Q , consider Figure 1.3, where we focus attention on the three yttrium atoms in the unit cell. Notice that the β^+ domain, if rotated 180 degrees about an axis parallel to the plane of the page, becomes the β^- domain. This rotation is a symmetry of the parent group which is not present in the child. Furthermore, the γ^+ domain, if rotated along the exact same axis, becomes the γ^- domain. If a crystal had a domain boundary between the β^+ and γ^- domains, the boundary energy would have to be the same as that between the β^- and γ^+ domains because their boundaries are equivalent by symmetry. In general, if a pair of domains can

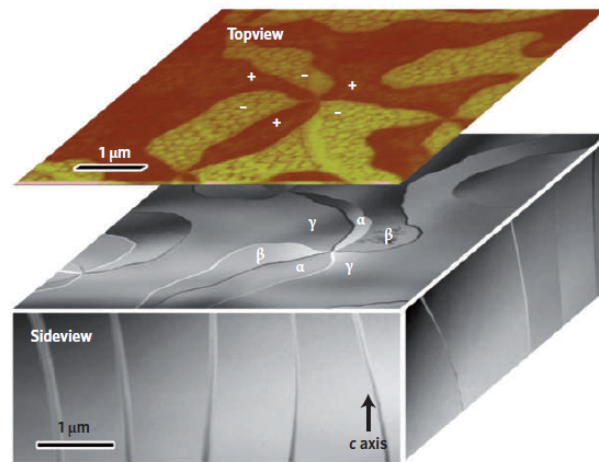


Figure 1.4 A ferroelectric map overlaid on an antiferroelectric map of $YMnO_3$. This shows that all six domains come together to form topological defects. [27]

be transformed into another pair of domains by a symmetry operation of the parent group, then their boundary energies must be identical. The action of G on the elements of Q is transitive, so that any domain can be permuted into any other domain. However, this action is not transitive over domain pairs. Some domain pairs are not related to one another by any permutation enacted by G . Because not all pairs are symmetrically equivalent, we can group domain pairs into equivalence classes (Figure 1.5).

Using this idea, a graph of the domain boundary energies can be made to help visualize how the domains might meet in a crystal. Because Q is isomorphic to three dimensional point group $6mm$ (Schönflies D_6 or abstract $D_3 \times \mathbb{Z}_2$), there is a natural way to embed the corresponding coset graph into the three-dimensional volume of the crystal. Assuming that the domain interfaces of one of the domain-pair equivalence classes will be energetically favorable relative to the others, we can select only the edges of that class from the coset graph to include in the embedding. In Figure 1.5, only the domain-pair equivalence class indicated by blue lines can yield the observed six-fold pinwheel pattern of Figure 1.4, wherein each domain favors interfaces with the two adjacement domains of

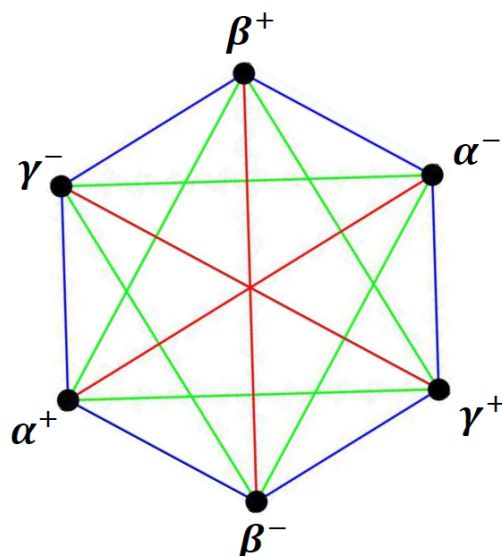


Figure 1.5 A domain graph of $YMnO_3$. Each black vertex represents a domain and each connecting line between vertices represents a domain pair, where color indicates the domain-pair equivalence class.

the pinwheel. The green class breaks up into two subclasses of three domains each, either one of which would yield a three-fold pinwheel; and the red class breaks up into three subclasses of two domains, any of which would yield only single planar domain boundary.

We envision using this same approach to characterize domain-boundary topology in any crystal that exhibits symmetry-lowering phase transitions. For any G and H (both space groups), find the normal core, $N_H(G)$, and the quotient group, $G/N_H(G)$, generate the coset graph, and employ it to better understand the possible domain-interface topologies that can result. Hence the need to know the normal subgroups of crystallographic space groups, which have not been exhaustively studied in previous work.

Chapter 2

Point Groups

2.1 Normal Subgroups and Quotients of Crystallographic Point Groups

The subgroups of each crystallographic point group are tabulated in the International Tables of Crystallography. [29] Our objective in this section is to identify each of the normal subgroups and to tabulate the corresponding quotient groups. That is, for a given subgroup $P_H \subseteq P_G$ we check to see if $gP_H = P_Hg$ for every $g \in P_G$. If this is satisfied then $P_H \trianglelefteq P_G$. Though not required for the derivation of normally supportive sublattices, point group quotients may prove to be useful in understanding the topology of defects in crystals. After finding the normal subgroups of a point group, it is not difficult to find the corresponding quotient group for each one.

Once we have tabulated every $P_N \trianglelefteq P_G$, we can then tabulate every $P_Q = P_G/P_N$. To do this for a given P_G and P_N , we first find the cosets of P_N in P_G by calculating gP_N with every $g \in P_G$. This group of cosets under coset multiplication is $P_Q = P_G/P_N$. Table 2.1 lists each crystallographic point group P_G and every cpg-normal subgroup P_N with the corresponding quotient group P_Q . Though the contents of Table 2.1 have, no doubt, been derived in the past, we're not aware of a

comparable presentation.

Since P_Q is the group of cosets of P_N in P_G , it is convenient to express P_Q as an isomorphic abstract group. To do this, we see how each element of P_Q permutes the elements of P_Q . We can then compare this permutation group to the permutation groups of the same order to find which groups are isomorphic. Table 2.2 lists the crystallographic point groups according to their isomorphism to abstract finite groups.

Tables 2.1 and 2.2 use symbols such as \mathbb{Z}_n and D_n to represent abstract groups. A brief explanation of each abstract group follows. \mathbb{Z}_n represents the cyclic group of order n , which is isomorphic to the set of integers 0 through $n - 1$ under addition modulo n . D_n is the dihedral group of order $2n$, which is isomorphic to the group of symmetries of a regular n -gon in two dimensions. A_n is the alternating group of degree n , which is isomorphic to the set of even permutations of n objects and has order $n!/2$. S_n is the symmetric group of degree n , which is isomorphic to the set of all permutations of n objects and has order $n!$.

Table 2.1 A table of normal subgroups of crystallographic point groups and corresponding quotient groups. The first column is the crystallographic point group P_G , the second column is a crystallographic point group that is a normal subgroup $P_N \trianglelefteq P_G$, the third column is an abstract group that is isomorphic to the quotient group $P_Q = P_G/P_N$. A subscript was added to the P_N symbol where needed to clarify which crystallographic axis corresponds to the normal subgroup.

P_G	P_N	P_Q	P_G	P_N	P_Q	P_G	P_N	P_Q	P_G	P_N	P_Q	P_G	P_N	P_Q
$\bar{1}$	1	\mathbb{Z}_2	4mm	1	D_4	321	1	D_3	622	1	D_6	6/mmm	3m1	D_2
2	1	\mathbb{Z}_2	4mm	2	D_2	321	3	\mathbb{Z}_2	622	2_z	D_3	6/mmm	31m	D_2
m	1	\mathbb{Z}_2	4mm	mm2	\mathbb{Z}_2	3m1	1	D_3	622	3	D_2	6/mmm	$\bar{3}1m$	\mathbb{Z}_2
2/m	1	D_2	4mm	4	\mathbb{Z}_2	3m1	3	\mathbb{Z}_2	622	312	\mathbb{Z}_2	6/mmm	$\bar{3}m1$	\mathbb{Z}_2
2/m	$\bar{1}$	\mathbb{Z}_2	$\bar{4}2m$	1	D_4	31m	1	D_3	622	321	\mathbb{Z}_2	6/mmm	6	D_2
2/m	2	\mathbb{Z}_2	$\bar{4}2m$	2_z	D_2	31m	3	\mathbb{Z}_2	622	6	\mathbb{Z}_2	6/mmm	$\bar{6}$	D_2
2/m	m	\mathbb{Z}_2	$\bar{4}2m$	222	\mathbb{Z}_2	$\bar{3}1m$	1	D_6	6mm	1	D_6	6/mmm	6/m	\mathbb{Z}_2
222	1	D_2	$\bar{4}2m$	$\bar{4}$	\mathbb{Z}_2	$\bar{3}1m$	$\bar{1}$	D_3	6mm	2_z	D_3	6/mmm	622	\mathbb{Z}_2
222	2	\mathbb{Z}_2	$\bar{4}m2$	1	D_4	$\bar{3}1m$	3	D_2	6mm	3	D_2	6/mmm	6mm	\mathbb{Z}_2
mm2	1	D_2	$\bar{4}m2$	2_z	D_2	$\bar{3}1m$	$\bar{3}$	\mathbb{Z}_2	6mm	3m1	\mathbb{Z}_2	6/mmm	$\bar{6}m2$	\mathbb{Z}_2
mm2	2	\mathbb{Z}_2	$\bar{4}m2$	mm2	\mathbb{Z}_2	$\bar{3}1m$	312	\mathbb{Z}_2	6mm	31m	\mathbb{Z}_2	6/mmm	$\bar{6}2m$	\mathbb{Z}_2
mmm	1	$D_2 \times \mathbb{Z}_2$	$\bar{4}m2$	$\bar{4}$	\mathbb{Z}_2	$\bar{3}1m$	31m	\mathbb{Z}_2	6mm	6	\mathbb{Z}_2	23	1	A_4
mmm	$\bar{1}$	D_2	4/mmm	1	$D_4 \times \mathbb{Z}_2$	$\bar{3}m1$	1	D_6	$\bar{6}m2$	1	D_6	23	222	\mathbb{Z}_3
mmm	2	D_2	4/mmm	$\bar{1}$	D_4	$\bar{3}m1$	$\bar{1}$	D_3	$\bar{6}m2$	m_z	D_3	$m\bar{3}$	1	$A_4 \times \mathbb{Z}_2$
mmm	m	D_2	4/mmm	2_z	$D_2 \times \mathbb{Z}_2$	$\bar{3}m1$	3	D_2	$\bar{6}m2$	3	D_2	$m\bar{3}$	$\bar{1}$	A_4
mmm	2/m	\mathbb{Z}_2	4/mmm	m_z	D_4	$\bar{3}m1$	$\bar{3}$	\mathbb{Z}_2	$\bar{6}m2$	312	\mathbb{Z}_2	$m\bar{3}$	222	\mathbb{Z}_6
mmm	222	\mathbb{Z}_2	4/mmm	2/m $_z$	D_2	$\bar{3}m1$	321	\mathbb{Z}_2	$\bar{6}m2$	3m1	\mathbb{Z}_2	$m\bar{3}$	mmm	\mathbb{Z}_3
mmm	mm2	\mathbb{Z}_2	4/mmm	222	D_2	$\bar{3}m1$	3m1	\mathbb{Z}_2	$\bar{6}m2$	$\bar{6}$	\mathbb{Z}_2	$m\bar{3}$	23	\mathbb{Z}_2
4	1	\mathbb{Z}_4	4/mmm	mm2 $_z$	D_2	6	1	\mathbb{Z}_6	$\bar{6}2m$	1	D_6	432	1	S_4
4	2	\mathbb{Z}_2	4/mmm	mmm	\mathbb{Z}_2	6	2	\mathbb{Z}_3	$\bar{6}2m$	m_z	D_3	432	222	D_3
$\bar{4}$	1	\mathbb{Z}_4	4/mmm	4	D_2	6	3	\mathbb{Z}_2	$\bar{6}2m$	3	D_2	432	23	\mathbb{Z}_2
$\bar{4}$	2	\mathbb{Z}_2	4/mmm	$\bar{4}$	D_2	$\bar{6}$	1	\mathbb{Z}_6	$\bar{6}2m$	321	\mathbb{Z}_2	$\bar{4}3m$	1	S_4
4/m	1	$\mathbb{Z}_4 \times \mathbb{Z}_2$	4/mmm	4/m	\mathbb{Z}_2	$\bar{6}$	m	\mathbb{Z}_3	$\bar{6}2m$	31m	\mathbb{Z}_2	$\bar{4}3m$	222	D_3
4/m	$\bar{1}$	\mathbb{Z}_4	4/mmm	422	\mathbb{Z}_2	$\bar{6}$	3	\mathbb{Z}_2	$\bar{6}2m$	$\bar{6}$	\mathbb{Z}_2	$\bar{4}3m$	23	\mathbb{Z}_2
4/m	2	D_2	4/mmm	4mm	\mathbb{Z}_2	6/m	1	$\mathbb{Z}_6 \times \mathbb{Z}_2$	6/mmm	1	$D_6 \times \mathbb{Z}_2$	$m\bar{3}m$	1	$S_4 \times \mathbb{Z}_2$
4/m	m	\mathbb{Z}_4	4/mmm	$\bar{4}2m$	\mathbb{Z}_2	6/m	$\bar{1}$	\mathbb{Z}_6	6/mmm	$\bar{1}$	D_6	$m\bar{3}m$	$\bar{1}$	S_4
4/m	2/m	\mathbb{Z}_2	4/mmm	$\bar{4}m2$	\mathbb{Z}_2	6/m	2	\mathbb{Z}_6	6/mmm	2_z	D_6	$m\bar{3}m$	222	D_6
4/m	4	\mathbb{Z}_2	3	1	\mathbb{Z}_3	6/m	m	\mathbb{Z}_6	6/mmm	m_z	D_6	$m\bar{3}m$	mmm	D_3
4/m	$\bar{4}$	\mathbb{Z}_2	$\bar{3}$	1	\mathbb{Z}_6	6/m	2/m	\mathbb{Z}_3	6/mmm	2/m $_z$	D_3	$m\bar{3}m$	23	D_2
422	1	D_4	$\bar{3}$	$\bar{1}$	\mathbb{Z}_3	6/m	3	D_2	6/mmm	3	$D_2 \times \mathbb{Z}_2$	$m\bar{3}m$	$m\bar{3}$	\mathbb{Z}_2
422	2_z	D_2	$\bar{3}$	3	\mathbb{Z}_2	6/m	$\bar{3}$	\mathbb{Z}_2	6/mmm	$\bar{3}$	D_2	$m\bar{3}m$	432	\mathbb{Z}_2
422	222	\mathbb{Z}_2	312	1	D_3	6/m	6	\mathbb{Z}_2	6/mmm	312	D_2	$m\bar{3}m$	$\bar{4}3m$	\mathbb{Z}_2
422	4	\mathbb{Z}_2	312	3	\mathbb{Z}_2	6/m	$\bar{6}$	\mathbb{Z}_2	6/mmm	321	D_2			

Table 2.2 A table of abstract groups and all the crystallographic point groups that are isomorphic to each.

Order	Abstract Groups	Isomorphic Point Groups
1	\mathbb{Z}_1	1
2	$\mathbb{Z}_2 \cong D_1$	$\bar{1} \cong 2 \cong m$
3	\mathbb{Z}_3	3
4	$D_2 \cong \mathbb{Z}_2 \times \mathbb{Z}_2$	$222 \cong mm2 \cong 2/m$
4	\mathbb{Z}_4	$4 \cong \bar{4}$
6	D_3	$312 \cong 31m$
6	$\mathbb{Z}_6 \cong \mathbb{Z}_3 \times \mathbb{Z}_2$	$\bar{3} \cong 6 \cong \bar{6}$
8	$D_2 \times \mathbb{Z}_2 \cong \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	mmm
8	D_4	$422 \cong 4mm \cong \bar{4}2m$
8	$\mathbb{Z}_4 \times \mathbb{Z}_2$	4/m
12	$D_6 \cong D_3 \times \mathbb{Z}_2$	$\bar{3}1m \cong 622 \cong 6mm \cong \bar{6}m2$
12	A_4	23
12	$\mathbb{Z}_6 \times \mathbb{Z}_2$	6/m
16	$D_4 \times \mathbb{Z}_2$	4/mmm
24	$A_4 \times \mathbb{Z}_2$	$m\bar{3}$
24	S_4	$432 \cong \bar{4}3m$
24	$D_6 \times \mathbb{Z}_2$	6/mmm
48	$S_4 \times \mathbb{Z}_2$	$m\bar{3}m$

Chapter 3

Normally Supportive Sublattices

3.1 The Hermite Normal Form of a Sublattice Basis

All matrices and vectors presented in this work are defined in the primitive parent setting, where the elements of T_G can be represented as elements of \mathbb{Z}^3 (the set of all integer triplets). Any sublattice $T_N \subseteq T_G$ can then be represented as an integer matrix in Hermite normal form:

$$B_N = \begin{pmatrix} B_{11} & 0 & 0 \\ B_{21} & B_{22} & 0 \\ B_{31} & B_{32} & B_{33} \end{pmatrix} \quad (3.1)$$

where the columns of B_N are basis vectors of the sublattice T_N , and $0 < \{B_{11}, B_{22}, B_{33}\}$, $0 \leq B_{21} < B_{22}$, and $0 \leq \{B_{31}, B_{32}\} < B_{33}$. The sublattice T_N is then the set of translations $\{B_N t_g | t_g \in \mathbb{Z}^3\}$.

There are an infinite number of possible bases that span any given lattice, however each set of basis vectors will reduce to the same Hermite normal form matrix. By searching for a representation of T_N in Hermite normal form, we are guaranteeing that each unique solution will represent a unique T_N .

3.2 Normally Supportive Conditions

For a given parent space group G , tabulating all of the possible normal subgroups of the point group $P_N \trianglelefteq P_G$ is not difficult since P_G is finite [29]. Because any translation group is abelian, all elements of T_G commute, and any possible sublattice T_N of T_G will be a normal subgroup of T_G . However, a given $P_N \trianglelefteq P_G$ and an arbitrary $T_N \trianglelefteq T_G$ may not be compatible for the purpose of generating subgroups of G , let alone normal subgroups of G [21]. Because of this, we need to apply some restrictions on the form that T_N can take.

In the setting of the parent lattice, each space group element can be expressed as a block affine matrix in the form

$$g = \begin{pmatrix} p_g & t_g \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} p_g & f_g + u_g + v_g \\ 0 & 1 \end{pmatrix} \in G \quad (3.2)$$

where $p_g \in P_G$ is a 3×3 matrix representing the point component and t_g is a 3×1 vector representing the translational component. The translation can be broken into three parts. The first part is a sublattice translation $v_g \in T_N$. The second part is a parent lattice translation $u_g \in T_G$ that lies within the unit cell of the sublattice (i.e. within the parallelepiped formed by the column vectors of B_N). The third part is a fractional translation f_g that accommodates glide planes and screw axes.

Let us assume that $N \trianglelefteq G$ and see what restrictions on T_N result. Since normality requires $ghg^{-1} \in N$ for every $h \in N$ and $g \in G$, let us consider a g that is simply a translation of the parent lattice. For any $u_g + v_g \in T_G$ and any $p_h \in P_N$ it follows that

$$\begin{pmatrix} E & u_g + v_g \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p_h & t_h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E & -(u_g + v_g) \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} p_h & -p_h(u_g + v_g) + t_h + u_g + v_g \\ 0 & 1 \end{pmatrix} \in N. \quad (3.3)$$

However since

$$\begin{pmatrix} p_h & t_h \\ 0 & 1 \end{pmatrix} \in N, \quad (3.4)$$

it follows that $u_g + v_g - p_h(u_g + v_g) \in T_N$ which can be rearranged as

$$(E - p_h)(u_g + v_g) \in T_N. \quad (3.5)$$

Furthermore for any $v_h \in T_N$, normality requires that

$$\begin{pmatrix} p_g & t_g \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E & v_h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p_g^{-1} & -p_g^{-1}t_g \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} E & p_g v_h \\ 0 & 1 \end{pmatrix} \in N \quad (3.6)$$

and thus

$$p_g v_h \in T_N. \quad (3.7)$$

It's important to recognize that applying B_N^{-1} to every $v_h \in T_N$ yields the set of all integer triplets: $\{B_N^{-1}v_h | v_h \in T_N\} = \mathbb{Z}^3$. Thus, we can multiply equation 3.5 on the left side by B_N^{-1} to obtain

$$B_N^{-1}(E - p_h)(u_g + v_g) \in \mathbb{Z}^3. \quad (3.8)$$

Equation 3.8 holds for every possible translation $u_g + v_g$, which runs over all of \mathbb{Z}^3 . Only an integer matrix can transform every triplet in \mathbb{Z}^3 to \mathbb{Z}^3 . Thus, equation 3.8 requires that

$$B_N^{-1}(E - p_h) \in \mathbb{Z}^{3 \times 3} \quad (3.9)$$

where $\mathbb{Z}^{3 \times 3}$ is the set of all 3×3 integer matrices.

Similarly we can multiply equation 3.7 on the left by B_N^{-1} to get $B_N^{-1}p_g v_h \in \mathbb{Z}^3$ or equivalently

$$(B_N^{-1}p_g B_N)(B_N^{-1}v_h) \in \mathbb{Z}^3 \quad (3.10)$$

and since $B_N^{-1}v_h$ can be any integer triplet then we must have

$$B_N^{-1}p_g B_N \in \mathbb{Z}^{3 \times 3}. \quad (3.11)$$

For convenience, we refer to this condition as P_G -invariance. To support the normality condition, the basis of the sublattice must satisfy both equation 3.9 and equation 3.11 for every $p_h \in P_N$ and every $p_g \in P_G$.

The focus of the present thesis, for a given G and P_N , is to identify all B_N that satisfy both equations 3.9 and 3.11 simultaneously. When B_N satisfies both equations, we refer to the corresponding sublattice T_N as “normally supportive” because it is capable of supporting an extension N of P_N by T_N that is normal in G . This doesn’t necessarily mean that such a normal extension will exist, only that its existence is not prevented by equations 3.9 and 3.11.

One might imagine solving equations 3.9 and 3.11 separately, and then taking the intersection of their solution spaces. However, equation 3.11 by itself generally results in a very difficult system of Diophantine equations. Thus, we first use equation 3.9, which is straightforward to apply, to narrow the candidate forms of B_N , and only then apply equation 3.11 to each candidate form in order to further restrict the solution space of B_N . In the special case that $P_N = \{e\}$, equation 3.9 becomes trivial, thus leaving us to solve equation 3.11 alone, which does not lend itself to the computational tools used in this work and which would be impractical to treat by hand for every crystallographic space group G . Instead, such a case can be handled by a numerical approach that identifies all normally supportive B_N up to a fixed supercell (i.e. sublattice unit cell) volume rather than determining all of the possibilities. [30]

3.3 Inclusion Sublattices

Here, we introduce another way of thinking about equation 3.9. Consider the group commutator of a lattice translation element $t_g \in T_G$ and a point group element $p_h \in P_N$, which is calculated as

$$\begin{pmatrix} E & t_g \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p_h & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E & -t_g \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p_h^{-1} & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} E & (E - p_h)t_g \\ 0 & 1 \end{pmatrix}. \quad (3.12)$$

By the conditions of normality, p_h is conjugated by t_g into another element of N whose point part is p_h , which is then right-multiplied by p_h^{-1} to obtain a pure translation that must be included in N . Or in other words, $(E - p_h)t_g \in T_N$ which is equivalent to equation 3.9 when t_g is cycled over

all of \mathbb{Z}^3 . However, the restrictions imposed on B_N are the same if we merely cycle t_g over the generators of \mathbb{Z}^3 , which generators are just the columns of the identity matrix. Our alternative to equation 3.9 then reduces to the statement that every row vector of $E - p_h$ for each $p_h \in P_N$ must be included in T_N . For this reason, we refer to these row vectors loosely as “inclusion vectors”. In general, the set of all row vectors obtained from each of the matrices $E - p_h$ result in some redundancy; in our implementation, we employ lattice-basis reduction to obtain a minimal set of inclusion vectors, which form the basis of an “inclusion sublattice” $T'_N \subseteq T_N$. The restrictions on B_N are then precisely those that allow only those sublattices T_N that contain T'_N .

The inclusion sublattice depends only upon the form of the operators $p_h \in P_N$ in the primitive parent setting, which in turn depend upon the lattice-centering type of G . When we consider all of the possibilities, we find 129 unique combinations of a parent lattice-centering type and a cpg-normal subgroup. We applied equation 3.9 to each of these 129 combinations and found only 41 unique inclusion sublattices, as detailed in Table 3.1. Thus, for any choice of G and P_N , the restrictions imposed on B_N from equation 3.9 will be identified with one of the 41 inclusion sublattices in this table. The actual restriction is that $B_N^{-1}b \in \mathbb{Z}^3$ for each basis vector b in the inclusion sublattice.

Table 3.1 A table of the unique inclusion sublattice bases. The first column is an integer index for convenience. The second column contains unique inclusion sublattice bases, where each row is a single basis vector. The third column lists each of the pairs of parent lattice-centering type and cpg-normal subgroup that share the same inclusion sublattice. The 39th inclusion sublattice, for example, lists 15 of such pairs.

	Inclusion sublattice	P_N with corresponding centering type
1	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	A C F I P R 1 1 1 1 1 1
2	$\begin{pmatrix} 0 & 0 & 2 \end{pmatrix}$	C P m_z m_z
3	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix}$	A m_y

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Table 3.1 – continued from previous page

	Inclusion vectors	P_N with corresponding centering type
4	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix}$	I m_x
5	$\begin{pmatrix} 0 & 2 & 0 \end{pmatrix}$	P m_y
6	$\begin{pmatrix} 1 & -1 & -1 \end{pmatrix}$	F m_x
7	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix}$	C m_x
8	$\begin{pmatrix} 1 & -1 & 1 \end{pmatrix}$	F m_y
9	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix}$	I m_y
10	$\begin{pmatrix} 1 & 1 & -1 \end{pmatrix}$	F m_z
11	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix}$	C I $m_y m_z$
12	$\begin{pmatrix} 2 & 0 & 0 \end{pmatrix}$	A P $m_x m_x$
13	$\begin{pmatrix} -1 & 1 & 0 \\ 1 & 1 & 2 \end{pmatrix}$	I I $2_z mm2_d$
14	$\begin{pmatrix} -1 & 1 & 0 \\ 1 & 2 & 0 \end{pmatrix}$	P P 3 $31m$
15	$\begin{pmatrix} 0 & 1 & -1 \\ 2 & 0 & 0 \end{pmatrix}$	A A $2_z mm2_z$
16	$\begin{pmatrix} 0 & 1 & -1 \\ 2 & 1 & 1 \end{pmatrix}$	I 2_x
17	$\begin{pmatrix} 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	P P $2_x mm2_x$

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Table 3.1 – continued from previous page

	Inclusion vectors	P_N with corresponding centering type
18	$\begin{pmatrix} 1 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	C C 2_y $mm2_y$
19	$\begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & 1 \end{pmatrix}$	F F 2_z $mm2_z$
20	$\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix}$	R R 3 $3m1$
21	$\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \end{pmatrix}$	I $mm2_y$
22	$\begin{pmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \end{pmatrix}$	I 2_y
23	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	P P P $3m1$ 6 $6mm$
24	$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix}$	I $mm2_x$
25	$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$	I I I 4 $4mm$ $mm2_z$
26	$\begin{pmatrix} 1 & 1 & -1 \\ -1 & 1 & -1 \end{pmatrix}$	F F 2_x $mm2_x$
27	$\begin{pmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \end{pmatrix}$	F F 2_y $mm2_y$

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Table 3.1 – continued from previous page

Inclusion vectors	P_N with corresponding centering type
28 $\begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \end{pmatrix}$	C P P P $mm2_z$ 4 $4mm$ $mm2_d$
29 $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	C C 2_x $mm2_x$
30 $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	P P 2_y $mm2_y$
31 $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \end{pmatrix}$	C P P 2_z 2_z $mm2_z$
32 $\begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \\ 2 & 1 & 1 \end{pmatrix}$	I I I I I 222 23 $\bar{4}$ $\bar{4}2m$ $\bar{4}3m$
33 $\begin{pmatrix} -1 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	P P P 321 $\bar{6}$ $\bar{6}2m$
34 $\begin{pmatrix} 0 & 1 & 1 \\ 0 & -1 & 1 \\ 2 & 0 & 0 \end{pmatrix}$	I $2/m_x$
35 $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	F F F F F 23 432 $\bar{4}3m$ $m\bar{3}$ $m\bar{3}m$

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Table 3.1 – continued from previous page

Inclusion vectors	P_N with corresponding centering type
36 $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{matrix} P & P & P & P & P & P & P & P \\ \bar{3} & 312 & \bar{3}1m & \bar{3}m1 & 622 & 6/m & \bar{6}m2 & 6/mmm \end{matrix}$
37 $\begin{pmatrix} 1 & 0 & 1 \\ -1 & 0 & 1 \\ 0 & 2 & 0 \end{pmatrix}$	$\begin{matrix} I \\ 2/m_y \end{matrix}$
38 $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \end{pmatrix}$	$\begin{matrix} I & I & I & I & I & I & I & I \\ 422 & 432 & 4/m & \bar{4}m2 & 4/mmm & m\bar{3} & m\bar{3}m & mmm \\ P & P & P & P & P & R & R & R \\ 23 & 432 & \bar{4}3m & m\bar{3} & m\bar{3}m & \bar{3} & 321 & \bar{3}m1 \end{matrix}$
39 $\begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{matrix} C & C & C & C & I & I & I & P \\ 222 & 2/m_x & 2/m_y & mmm & 222_d & 2/m_z & mmm_d & 222_d \\ P & P & P & P & P & P & P \\ \bar{4} & 422 & \bar{4}2m & 4/m & \bar{4}m2 & 4/mmm & mmm_d \end{matrix}$
40 $\begin{pmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$	$\begin{matrix} F & F & F & F & F \\ 222 & 2/m_x & 2/m_y & 2/m_z & mmm \end{matrix}$
41 $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$\begin{matrix} C & C & F & I & P & P & P & P & P & P & R \\ \bar{1} & 2/m_z & \bar{1} & \bar{1} & \bar{1} & 222 & 2/m_x & 2/m_y & 2/m_z & mmm & \bar{1} \end{matrix}$

3.4 The Extension Problem

Because the fractional translation f_g of each space group element is fixed by the choice of parent space group G , and the point operators p_h are fixed by the choice of P_N , only the u translations remain to be determined. Any set of u translations that yields a valid subgroup (i.e. results in a set of operators that obey the same multiplication table as those of P_N under multiplication modulo T_N) is an extension of P_N by T_N in G . Because the u_h translation of any p_h must be contained within the unit cell of the sublattice, there are only a finite number of ways to assign u translations to each of the point operators, most of which will not result in subgroups. When a set of u translations does yield a subgroup of G , that subgroup is a space group from the same arithmetic crystal class as G (they are extensions of the same non-symmorphic group). In the remainder of this section, we will assume that the u translations have already been restricted so that the extension N of P_N by T_N is a valid subgroup of G .

In general, normality of N in G requires that $r = ghg^{-1} \in N$ for every $h \in N$ and $g \in G$. We can express this in affine matrix form as

$$\begin{pmatrix} p_r & f_r + u_r + v_r \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} p_g & f_g + u_g + v_g \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p_h & f_h + u_h + v_h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p_g^{-1} & -p_g^{-1}(f_g + u_g + v_g) \\ 0 & 1 \end{pmatrix}. \quad (3.13)$$

After expanding the product in equation 3.13, the point part reduces to

$$p_r = p_g p_h p_g^{-1} \quad (3.14)$$

and the translational part reduces to

$$f_r + u_r + v_r = (E - p_r)(f_g + u_g + v_g) + p_g(f_h + u_h + v_h). \quad (3.15)$$

Equation 3.14 merely requires that $P_N \trianglelefteq P_G$, which is obvious. Since $v_r \in T_N$, we can rearrange equation 3.15 as

$$v_r = [(E - p_r)f_g + p_g(f_h + u_h) - (f_r + u_r)] + (E - p_r)(u_g + v_g) + p_g v_h \in T_N. \quad (3.16)$$

From equations 3.5, 3.7, and 3.16, it follows that

$$(E - p_r)f_g + p_g(f_h + u_h) - (f_r + u_r) \in T_N. \quad (3.17)$$

Equation 3.17 will be satisfied if and only if extension N of P_N by T_N is normal in G . Again, we emphasize that for some normally supportive sublattices T_N of G with P_N , it may be that none of the extensions of P_N by T_N in G will be normal in G . Thus some of the normally supportive sublattices obtained using the method described in the preceding sections may not actually support any normal extensions. But the sublattice of any csg-normal subgroup of G must be normally supportive. Furthermore, because equations 3.9 and 3.11 do not involve the translational parts of the space-group operators, the normally-supportive sublattices T_N with P_N of two space groups G_1 and G_2 will be the same so long as G_1 and G_2 belong to the same arithmetic crystal class.

Chapter 4

Algorithm

4.1 Overview

With a given point group P_G and a normal subgroup $P_N \trianglelefteq P_G$, the first step is to apply equation 3.9 with each $p_h \in P_N$ to find constraints on B_N . In general, each element of the matrix that results from the product on the left hand side of equation 3.9 can be a complicated rational expression containing all of the elements of B_N . Each of the matrix elements for each of the $p_n \in P_N$ must simultaneously take on integer values in order to satisfy the equation. We used Mathematica's built-in Reduce command to apply the integer restrictions and thereby find the values that the entries of B_N can take.

Next, starting with the restricted form of B_N resulting from equation 3.9, we do a similar thing with the much more difficult equation 3.11, where the elements of the matrix products for all $p_g \in P_G$ must simultaneously take on integer values. Of these terms, we are only interested in the ones that are not obviously integers. That is, we are interested in the terms with quotients. Again, we can use Mathematica's Reduce command to apply the integer-value restriction, and thereby obtain the restricted forms of B_N that satisfy both equations 3.9 and 3.11. There are some quotient

terms that are too complicated for Mathematica's built in reduction features. When this is the case, we simply keep track of these quotients and include the requirement that they be integral as extra conditions.

Because the normally supportive sublattices are identical for every space group in a given arithmetic crystal class, we organize our output according to the 73 arithmetic crystal classes, each of which is represented by its unique symmorphic space-group G . For a given G and cpg-normal subgroup P_N , the output of our algorithm is a set of triplets, where the symmetry-restricted form of B_N itself is the second part of each triplet. The first part of each triplet contains a list of inequalities that indicate the range of each variable in the corresponding B_N matrix (this part is empty if there are no variables in B_N). The third part of each triplet contains any additional quotient expressions that must have integer values. In most cases, it was possible to achieve a standard form for the triplet in which the range of each variable is the set of all non-negative integers. The full set of triplets should collectively span the space of all normally supportive sublattices T_N of G with P_N . And all triplets should be mutually disjoint so as to entirely avoid redundancies.

4.2 Subroutines

The essential challenge with each of the many processing steps that we applied to the Mathematica's Reduce output was to modify the symbolic form of B_N and its conditions without altering the solution space that they represent (i.e. the space of normally supportive sublattices). Thus every step of the processing yields a correct form but not necessarily a form that looks nice or is easy to understand. This effort required considerable attention to detail.

Depending on the specific case, the output from Reduce can take on a variety of different forms. A major component of the present research effort was devoted to bringing the output to a uniform format that follows relatively nice rules. First, simple steps were taken to extract information

about the B_N matrix and the conditions on its elements, eliminate special conditions that were obviously true, simplify complicated logical statements, and separate joint statements into lists of simultaneous conditions. A number of subroutines were then developed in order to further shape the output, each one handling a specific issue. We describe each subroutine below, where each paragraph begins with the name of the subroutine in quotes for easy reference to the Mathematica code.

The "relabelvars" module was used to relabel variables for convenience. To make each triplet look uniform, each variable is presented in the form of a letter combined with a number. Each variable that appears in an extra condition is denoted as d_n while all the other variables are denoted as c_n where n is an integer. Each variable is then numbered in the order that it appears in the B_N matrix, starting from the top and left side and proceeding row by row with the c variables and d variables numbered separately (i.e. a triplet can contain both c_1 and d_1). Because many of the subroutines introduce new variables into the triplets they modify, it was convenient to periodically relabel all of the variables in a triplet in a uniform way during the multi-step reduction process.

The "eliminatesimpleton" module was used to get rid of simple extra conditions. The extra conditions often took the form of an integer divided by a lone variable. To simplify this, we set the variable to a divisor of the numerator. Doing this can have multiple solutions when the numerator has multiple divisors. In such a case, the triplet bifurcates into multiple less complicated triplets, one for each solution.

The "removequotients" module was used to make the B_N matrices look nicer. Sometimes the output of Reduce leaves quotients in the B_N matrix. Since each B_N must be in Hermite normal form, its entries must all be integers. For this reason, it was convenient to replace such a quotient with a new variable in B_N , and then solve for one of the other variables, adding the resulting quotient to the list of extra conditions in the last portion of the triplet.

The "cleanuptriplet" module was used to eliminate obvious extra conditions. Most of these

subroutines aim to simplify the extra conditions, which sometimes leaves extra conditions that are unnecessary, redundant, or sometimes even impossible to satisfy. In the event that a triplet contains an extra condition that cannot possibly be an integer, such as $d_2 + \frac{1}{2}$, it does not represent any possible normally supportive sublattices, and thus the entire triplet can be deleted. In the event that an extra condition is obviously an integer, e.g. 2 , $d_1 + 1$, $2d_2(1 - d_2)$, etc., we needn't keep track of it and thus it can be removed from the list of extra conditions. In the event that two extra conditions are linearly dependent, for example $\frac{1-d_3^2}{2}$ and $\frac{1-d_3^2}{2d_2}$, the less restricting of the two ($\frac{1-d_3^2}{2}$ in our example) is redundant and can be removed from the list of extra conditions. This module is implemented frequently because many of the other subroutines change the extra conditions so as to leave cases that can be cleaned up.

The "hyperreduce" module was used to simplify variable ranges. After removing the quotients from the B_N matrices, some quotients are introduced into the conditions. This often tends to make the ranges on variables very complicated. To remedy this, we again use the Reduce command, but this time only on the obviously complicated conditions. This step sometimes has the side effect of making a single triplet split into multiple but nicer looking triplets.

The "eliminatefractional" module was used to simplify certain extra conditions. Sometimes there are extra conditions in the form $\frac{n_1}{n_2}d$ where d is a variable in the B_N matrix and n_1 and n_2 are integers. This can be simplified a little because the only values of d that will satisfy this condition are multiples of n_2 . If we simply let $h = d/n_2$, then we can replace all instances of d in the triplet with n_2h and thus we will have one less extra condition in these cases (the h will then be relabeled as a new c or d variable).

The "replaceprettyuglies" module was used to simplify some of the nicer looking extra conditions. Sometimes there are extra conditions where a variable appears only once in the numerator of an extra condition. In other words, the extra condition has the form $\frac{polynomial_1 + nd}{polynomial_2}$ where n is a constant integer, d is a variable in the B_N matrix and the *polynomials* do not contain the variable d .

This condition can be eliminated with a little work. If we let $\frac{\text{polynomial}_1 + nd}{\text{polynomial}_2} = k$ then we can replace all instances of d in the triplet with $\frac{1}{n}(k\text{polynomial}_2 - \text{polynomial}_1)$ which will eliminate this extra condition (k will then be relabeled as a new c or d variable). The standard form doesn't allow any variable expression in B_N that are not obviously integers. To avoid introducing numerical fractions in B_N in this step, we make a second replacement to remove any $\frac{1}{n}$ that might appear in the triplet.

The "eliminatedependentvars" module was used to restrict the number of variables to a minimum. Sometimes the output of Reduce gives more variables than is necessary. For example, a particular B_N matrix might have only three elements with variables which have the form $2(3 + d_1 + d_2 + d_3)$, $2(4 + d_1 + 2d_2)$, and $4(3 + d_1 + d_2 + d_3)$. By inspection it can be seen that the third element is exactly double the first element and thus there are only two linearly independent polynomials. This is a problem because there are three variables to span B_N which means that there are redundancies. The desired format is by definition free of variable redundancies – it doesn't permit more than one set of variable values to achieve the same numerical B_N matrix. To fix this problem, it was necessary to rewrite these polynomials in terms of only two variables that span the same B_N space. To do this we implemented Mathematica's GroebnerBasis command which takes a series of polynomials and returns a set of linearly independent polynomials that span the same space. In the example above, the Gröbner basis is $\{d_2 - d_3, d_1 + 2d_3\}$. If we let $f_1 = d_2 - d_3$ and $f_2 = d_1 + 2d_3$ then we can replace every instance of d_1 with $f_2 - 2d_3$ and every instance of d_2 with $f_1 + d_3$ then the original expressions above become $2(3 + f_1 + f_2)$, $2(1 + 2f_1 + f_2)$, and $4(3 + f_1 + f_2)$ which has only two variables; the f variables will then be relabeled as c or d variables.

The "removeexcesscondvars" module was used to get rid of unnecessary conditions on the ranges of the variables. While the eliminatedependentvars routine does an excellent job at removing unnecessary variables in the B_N matrices, it fails to reduce the corresponding number of variables in the list of conditions. To illustrate this problem, consider the example in the previous

paragraph where d_1 , d_2 , and d_3 could be any non-negative integer. After replacing d_1 with $f_2 - 2d_3$ and d_2 with $f_1 + d_3$, our conditions become $f_2 - 2d_3 \geq 0$, $f_1 + d_3 \geq 0$, and $d_3 \geq 0$. It is no longer necessary to keep track of d_3 since it was eliminated from B_N , however d_3 is necessary to determine what values f_1 and f_2 can take. To eliminate d_3 from the conditions, we first isolate it in each inequality which $f_2/2 \geq d_3$, $d_3 \geq -f_1$, and $d_3 \geq 0$. We can then combine these three conditions into the following two compound inequalities $f_2/2 \geq d_3 \geq 0$ and $f_2/2 \geq d_3 \geq -f_1$. Since the value of d_3 makes no difference in B_N , we can choose to set it equal to the shared maximum value in both compound inequalities which then simplifies them to $f_2/2 \geq 0$ and $f_2/2 \geq -f_1$ and thus d_3 is now completely removed from the triplet. This module has the unfortunate side effect of leaving somewhat awkward conditions, which are later improved by the hyperreduce subroutine.

The order in which the subroutines were applied is somewhat strategic and somewhat arbitrary. Often, the application of one subroutine recreated undesirable structures within the matrix or conditions that were resolved by a previous subroutine, so that the first subroutine needed to be reapplied. This led to seemingly arbitrary iterations in the application of certain groups of subroutines. The specific and rather delicate ordering of subroutine calls that we ultimately converged on did bring all cases into the desired uniform format; but it is likely that other orderings might also accomplish this. However, we also point out some small and seemingly unimportant deviations from the specific ordering that we applied failed spectacularly to deliver the desired format.

Chapter 5

Results and Discussion

5.1 Tables

Normally supportive sublattices have been tabulated and are listed in appendix A. Many table entries contain a symbolic B_N matrix that actually represents an infinite family of sublattices. Table 5.1 is a summary of Table A.1 organized by arithmetic crystal class. The first column is an integer index for the 73 arithmetic crystal classes. The second column is the symmorphic crystallographic space group symbol that represents the arithmetic class. The third column is the total number of B_N matrices from all cpg-normal subgroups of the arithmetic class. The last column indicates the number of B_N families in square brackets associated with each cpg-normal subgroup of an arithmetic class.

There are a total of 1773 B_N families accounted for in Table 5.1. Keep in mind that some families are larger than others due to differences in dimensionality (i.e. the number of free variables of infinite range in the symbolic form). For a given cpg-normal subgroup, one three-dimensional B_N family is vastly larger than three zero-dimensional B_N families, but collectively equivalent in size to three one-dimensional B_N families. For example, ACC $R3$ (#39) lists only one cpg-

normal subgroup, which has only a single B_N family, which turns out to be a one-dimensional infinite family. ACC $P\bar{1}$ (#2), on the other hand, lists only one cpg-normal subgroup, which has 16 different B_N families, all of which turn out to be zero-dimensional (i.e. families containing one individual each).

Due to the exceptional complexity of most cases for which the cpg-normal subgroup is 1, all of these cases were excluded from the present work and tables, including the handful of cases that proved to be readily solvable using the present methods. As mentioned earlier, cases for which the npg-subgroup is 1 can be treated numerically by method of Morgan and Hart. [30]

Table 5.1 The number of families of normally-supportive sublattices for each arithmetic crystal class (ACC), and for each cpg-normal subgroup of each ACC.

ACC	total	cpg-normal subgroups and number of corresponding B_N families			
1 P1	–	–			
2 $P\bar{1}$	16	$\bar{1}$ [16]			
3 P2	11	2_z [11]			
4 C2	11	2_z [11]			
5 Pm	5	m_z [5]			
6 Cm	5	m_z [5]			
7 P2/m	48	$\bar{1}$ [16]	2_z [11]	m_z [5]	$2/m_z$ [16]
8 C2/m	48	$\bar{1}$ [16]	2_z [11]	m_z [5]	$2/m_z$ [16]
9 P222	49	2_x [11]	2_y [11]	2_z [11]	222[16]
10 C222	19	2_x [6]	2_y [3]	2_z [5]	222[5]
11 F222	15	2_x [4]	2_y [3]	2_z [3]	222[5]
12 I222	21	2_x [5]	2_y [5]	2_z [5]	222[6]
13 Pmm2	44	2_z [11]	m_x [11]	m_y [11]	$mm2_z$ [11]
14 Cmm2	14	2_z [5]	m_x [2]	m_y [4]	$mm2_z$ [3]
15 Amm2	85	2_z [3]	m_x [77]	m_y [2]	$mm2_z$ [3]
16 Fmm2	19	2_z [3]	m_x [2]	m_y [11]	$mm2_z$ [3]
17 Imm2	34	2_z [5]	m_x [7]	m_y [20]	$mm2_z$ [2]

Continued on next page

Table 5.1 – continued from previous page

ACC	total	cpg-normal subgroups and number of corresponding B_N families						
18 Pmmm	192	$\bar{1}[16]$	$2_x[11]$	$2_y[11]$	$2_z[11]$	$m_x[11]$	$m_y[11]$	$m_z[8]$
		$2/m_x[16]$	$2/m_y[16]$	$2/m_z[16]$	$222[16]$	$mm2_x[11]$	$mm2_y[11]$	$mm2_z[11]$
		$mmm[16]$						
19 Cmmm	77	$\bar{1}[8]$	$2_x[6]$	$2_y[3]$	$2_z[5]$	$m_x[2]$	$m_y[4]$	$m_z[9]$
		$2/m_x[5]$	$2/m_y[5]$	$2/m_z[8]$	$222[5]$	$mm2_x[6]$	$mm2_y[3]$	$mm2_z[3]$
		$mmm[5]$						
20 Fmmm	79	$\bar{1}[6]$	$2_x[4]$	$2_y[3]$	$2_z[3]$	$m_x[2]$	$m_y[11]$	$m_z[15]$
		$2/m_x[5]$	$2/m_y[5]$	$2/m_z[5]$	$222[5]$	$mm2_x[4]$	$mm2_y[3]$	$mm2_z[3]$
		$mmm[5]$						
21 Immm	83	$\bar{1}[6]$	$2_x[5]$	$2_y[5]$	$2_z[5]$	$m_x[7]$	$m_y[20]$	$m_z[12]$
		$2/m_x[3]$	$2/m_y[3]$	$2/m_z[3]$	$222[6]$	$mm2_x[2]$	$mm2_y[2]$	$mm2_z[2]$
		$mmm[2]$						
22 P4	8	$2_z[5]$	$4[3]$					
23 I4	7	$2_z[5]$	$4[2]$					
24 P $\bar{4}$	10	$2_z[5]$	$\bar{4}[5]$					
25 I $\bar{4}$	11	$2_z[5]$	$\bar{4}[6]$					
26 P4/m	42	$\bar{1}[8]$	$2_z[5]$	$m_z[8]$	$2/m_z[8]$	$4[3]$	$\bar{4}[5]$	$4/m[5]$
27 I4/m	34	$\bar{1}[4]$	$2_z[5]$	$m_z[12]$	$2/m_z[3]$	$4[2]$	$\bar{4}[6]$	$4/m[2]$
28 P422	26	$2_z[5]$	$222[8]$	$222_d[5]$	$4[3]$	$422[5]$		
29 I422	18	$2_z[5]$	$222[6]$	$222_d[3]$	$4[2]$	$422[2]$		
30 P4mm	19	$2_z[5]$	$mm2_z[5]$	$mm2_d[3]$	$4[3]$	$4mm[3]$		
31 I4mm	16	$2_z[5]$	$mm2_z[2]$	$mm2_d[5]$	$4[2]$	$4mm[2]$		
32 P $\bar{4}2m$	26	$2_z[5]$	$222[8]$	$mm2_d[3]$	$\bar{4}[5]$	$\bar{4}2m[5]$		
33 P $\bar{4}m2$	25	$2_z[5]$	$222_d[5]$	$mm2_z[5]$	$\bar{4}[5]$	$\bar{4}m2[5]$		
34 I $\bar{4}m2$	18	$2_z[5]$	$222_d[3]$	$mm2_z[2]$	$\bar{4}[6]$	$\bar{4}m2[2]$		
35 I $\bar{4}2m$	28	$2_z[5]$	$222[6]$	$mm2_d[5]$	$\bar{4}[6]$	$\bar{4}2m[6]$		
36 P4/mmm	107	$\bar{1}[8]$	$2_z[5]$	$m_z[16]$	$2/m_z[8]$	$222[8]$	$222_d[5]$	$mm2_z[5]$
		$mm2_d[3]$	$mmm[8]$	$mmm_d[5]$	$4[3]$	$\bar{4}[5]$	$4/m[5]$	$422[5]$

Continued on next page

Table 5.1 – continued from previous page

ACC	total	cpg-normal subgroups and number of corresponding B_N families						
36 P4/mmm	107	4mm[3]	$\bar{4}2m[5]$	$\bar{4}m2[5]$	4/mmm[5]			
37 I4/mmm	69	$\bar{1}[4]$	$2_z[5]$	$m_z[12]$	$2/m_z[3]$	222[6]	$222_d[3]$	$mm2_z[2]$
		$mm2_d[5]$	mmm[2]	$mmm_d[3]$	4[2]	$\bar{4}[6]$	4/m[2]	422[2]
		4mm[2]	$\bar{4}2m[6]$	$\bar{4}m2[2]$	4/mmm[2]			
38 P3	4	3[4]						
39 R3	1	3[1]						
40 P $\bar{3}$	10	$\bar{1}[4]$	3[4]	$\bar{3}[2]$				
41 R $\bar{3}$	7	$\bar{1}[4]$	3[1]	$\bar{3}[2]$				
42 P312	6	3[4]	312[2]					
43 P321	6	3[2]	321[4]					
44 R32	3	3[1]	321[2]					
45 P3m1	3	3[2]	3m1[1]					
46 P31m	8	3[4]	31m[4]					
47 R3m	2	3[1]	3m1[1]					
48 P $\bar{3}1m$	18	$\bar{1}[4]$	3[4]	$\bar{3}[2]$	312[2]	31m[4]	$\bar{3}1m[2]$	
49 P $\bar{3}m1$	15	$\bar{1}[4]$	3[2]	$\bar{3}[2]$	321[4]	3m1[1]	$\bar{3}m1[2]$	
50 R $\bar{3}m$	12	$\bar{1}[4]$	3[1]	$\bar{3}[2]$	321[2]	3m1[1]	$\bar{3}m1[2]$	
51 P6	5	$2_z[2]$	3[2]	6[1]				
52 P $\bar{6}$	13	$m_z[7]$	3[2]	$\bar{6}[4]$				
53 P6/m	28	$\bar{1}[4]$	$2_z[2]$	$m_z[7]$	$2/m_z[4]$	3[2]	$\bar{3}[2]$	6[1]
		$\bar{6}[4]$	6/m[2]					
54 P622	13	$2_z[2]$	3[2]	312[2]	321[4]	6[1]	622[2]	
55 P6mm	9	$2_z[2]$	3[2]	3m1[1]	31m[2]	6[1]	6mm[1]	
56 P $\bar{6}m2$	16	$m_z[5]$	3[2]	312[2]	3m1[1]	$\bar{6}[4]$	$\bar{6}m2[2]$	
57 P $\bar{6}2m$	21	$m_z[5]$	3[2]	321[4]	31m[2]	$\bar{6}[4]$	$\bar{6}2m[4]$	
58 P6/mmm	50	$\bar{1}[4]$	$2_z[2]$	$m_z[5]$	$2/m_z[4]$	3[2]	$\bar{3}[2]$	312[2]
		321[4]	3m1[1]	31m[2]	$\bar{3}1m[2]$	$\bar{3}m1[2]$	6[1]	$\bar{6}[4]$
		6/m[2]	622[2]	6mm[1]	$\bar{6}m2[2]$	$\bar{6}2m[4]$	6/mmm[2]	

Continued on next page

Table 5.1 – continued from previous page

ACC	total	cpg-normal subgroups and number of corresponding B_N families						
59 P23	6	222[4]	23[2]					
60 F23	3	222[2]	23[1]					
61 I23	12	222[6]	23[6]					
62 Pm $\bar{3}$	16	$\bar{1}$ [4]	222[4]	mmm[4]	23[2]	m $\bar{3}$ [2]		
63 Fm $\bar{3}$	9	$\bar{1}$ [3]	222[2]	mmm[2]	23[1]	m $\bar{3}$ [1]		
64 Im $\bar{3}$	19	$\bar{1}$ [3]	222[6]	mmm[2]	23[6]	m $\bar{3}$ [2]		
65 P432	8	222[4]	23[2]	432[2]				
66 F432	4	222[2]	23[1]	432[1]				
67 I432	14	222[6]	23[6]	432[2]				
68 P $\bar{4}3m$	8	222[4]	23[2]	$\bar{4}3m$ [2]				
69 F $\bar{4}3m$	4	222[2]	23[1]	$\bar{4}3m$ [1]				
70 I $\bar{4}3m$	18	222[6]	23[6]	$\bar{4}3m$ [6]				
71 Pm $\bar{3}m$	22	$\bar{1}$ [4]	222[4]	mmm[4]	23[2]	m $\bar{3}$ [2]	432[2]	$\bar{4}3m$ [2]
		m $\bar{3}m$ [2]						
72 Fm $\bar{3}m$	12	$\bar{1}$ [3]	222[2]	mmm[2]	23[1]	m $\bar{3}$ [1]	432[1]	$\bar{4}3m$ [1]
		m $\bar{3}m$ [1]						
73 Im $\bar{3}m$	29	$\bar{1}$ [3]	222[6]	mmm[2]	23[6]	m $\bar{3}$ [2]	432[2]	$\bar{4}3m$ [6]
		m $\bar{3}m$ [2]						

Consider the arithmetic class represented by crystallographic space group $Pmmm$ (#18 in Table 5.1) which has m_x , m_y , and m_z each listed as separate cpg-normal subgroups, where m_x and m_y both have 11 B_N families while m_z only has 8. Even the B_N families of m_x and m_y look very different; no numerical instance of one is contained in the other. Because m_x , m_y , and m_z are equivalent in some sense (they can be conjugate subgroups of the normalizer of $Pmmm$ with respect to Euclidean transformations), this is immediately surprising. The resolution of this paradox lies in the fact that B_N is presented as a column-HNF matrix, which is lower triangular so that the x , y and z basis vectors can have different numbers of non-zero values. Thus, while the B_N families of

these cpg-normal subgroups look very different, one can swap the first two rows of any numeric instance of B_N associated with m_x and reduce the result again to a column-HNF matrix to obtain the corresponding numerical instance of B_N associated with m_y .

Of the four cpg-normal subgroups of ACC *Amm2* (#15), cpg-normal subgroups 2_z , m_y , and $mm2_z$ each have 3 or fewer B_N families, while m_x has an impressive 77 B_N families. This latter cpg-normal subgroup proved exceptional in a variety of ways. Of the list of 74 unique conditions listed in Table A.2, this case alone contributes 24 of them, including the only 4 cases where negative variable values are allowed. ACCs that stood out amongst the others in terms of complexity were those based on point groups mmm , $4/mmm$, and $6/mmm$. Here, the large numbers of total B_N families per ACC arise due to large numbers of cpg-normal subgroups, and not because any one normal subgroup provides an extraordinary number of B_N families.

The B_N matrices of Table A.1 are all presented in the primitive HNF setting of the parent space group. To transform a B_N matrix from this table into the more familiar conventional setting, we multiply it on the left by the appropriate transformation matrix from the list below according to lattice-centering type (e.g. P, A, C, I, F, or R).

$$\begin{aligned}
 Q(P) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & Q(A) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix} & Q(C) &= \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
 Q(F) &= \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} & Q(I) &= \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} & Q(R) &= \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}
 \end{aligned} \tag{5.1}$$

As an example, if the sublattice basis in the primitive HNF setting of a face-centered cubic

parent lattice is

$$B_N = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1+c_1 & c_1 & 2+c_1 \end{pmatrix}, \quad (5.2)$$

the new basis in the conventional face-centered setting would be

$$Q(F)B_N = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1+c_1 & c_1 & 2+c_1 \end{pmatrix} = \begin{pmatrix} \frac{2+c_1}{2} & \frac{2+c_1}{2} & \frac{2+c_1}{2} \\ \frac{2+c_1}{2} & \frac{c_1}{2} & \frac{2+c_1}{2} \\ 1 & 1 & 0 \end{pmatrix}. \quad (5.3)$$

Obviously, this is no longer in Hermite normal form.

5.2 Validation

Extensive brute-force testing of Table A.1 helped us to identify and resolve problems with the computer algorithm. Though we have considerable confidence in the present table, we emphasize that it is only practical to run tests over a finite range of the infinite space of possible numerical B_N matrices. It is possible that a wider search would uncover problems that we have missed. For this reason, we will make our code publicly available. To verify the legitimacy of our output, we have performed the following three tests.

For the first test, a matrix is compared to the list of B_N matrices that have been tabulated. This matrix is also checked to see if it supports normality by checking if it satisfies equations 3.9 and 3.11. The matrix should fit one of our tabulated B_N forms if and only if it supports normality. If we find a matrix that fits one of our B_N forms but does not support normality or does not fit any form but does support normality then we know that there is an error in our tabulations. We have used this test with every possible Hermite normal form matrix with entries of values equal to or less than 6.

The second test focused on the variables in the B_N matrices. For each of our tabulated B_N , if there are no variables we simply check that it supports normality. If there are variables, we plug in values for those variables to make a matrix. The values that are plugged in are checked to see if they satisfy any extra conditions that the B_N has (if any) and the matrix is then checked to see if it supports normality. If there are any values that satisfy one but not the other then there is an error in our tabulations. We have applied this test plugging in every combination of values up to 50 for every one of our tabulated B_N matrices.

The third test focused on extra conditions and was not applied to any B_N that had no extra conditions. For each case, different values are plugged in for each variable in a systematic order until a combination of values that satisfy all extra conditions in a triplet are found. Then these values are plugged into the B_N matrix and it is checked that it supports normality. We have used this test to find every combination of values up to 250 that satisfy each set of extra conditions and verify that each solution satisfies normality. The results of this test were also used as a brute force method to check if there were even any solutions for each set of extra conditions (there were some cases that had no solutions or had a finite number of solutions).

Chapter 6

Examples

6.1 A Simple Case

Consider space group $P312$ (#149), the point group of which has six elements: $P_G = \{(x, y, z), (y, -x - y, z), (-x - y, x, z), (-y, -x, -z), (x + y, -y, -z), (-x, x + y, -z)\}$. P_G has three normal subgroups: $\{(x, y, z), (y, -x - y, z), (-x - y, x, z), (-y, -x, -z), (x + y, -y, -z), (-x, x + y, -z)\}$, $\{(x, y, z), (y, -x - y, z), (-x - y, x, z)\}$, and $\{(x, y, z)\}$. For this example, let us consider the normal subgroup $P_N = \{(x, y, z), (y, -x - y, z), (-x - y, x, z)\}$. The lattice-coordinate matrix representation of the elements of P_G is

$$\left\{ \begin{array}{l} \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{array} \right), \\ \left(\begin{array}{ccc} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{array} \right), \left(\begin{array}{ccc} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -1 \end{array} \right), \left(\begin{array}{ccc} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{array} \right) \end{array} \right\} \quad (6.1)$$

so that P_N is represented as

$$\left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}. \quad (6.2)$$

When we impose equation 3.9 on each of the point operators of P_N , the identity yields only trivial conditions, whereas the other two elements yield

$$B_N^{-1} \begin{pmatrix} 1 & 1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{B_{11}} & & 0 \\ -\frac{1}{B_{22}} - \frac{B_{21}}{B_{11}B_{22}} & \frac{2}{B_{22}} - \frac{B_{21}}{B_{11}B_{22}} & 0 \\ \frac{B_{32}}{B_{22}B_{33}} + \frac{-B_{22}B_{31}+B_{21}B_{32}}{B_{11}B_{22}B_{33}} & \frac{-2B_{32}}{B_{22}B_{33}} + \frac{-B_{22}B_{31}+B_{21}B_{32}}{B_{11}B_{22}B_{33}} & 0 \end{pmatrix} \in \mathbb{Z}^{3 \times 3} \quad (6.3)$$

and

$$B_N^{-1} \begin{pmatrix} 2 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{2}{B_{11}} & & 0 \\ \frac{1}{B_{22}} - \frac{2B_{21}}{B_{11}B_{22}} & \frac{1}{B_{22}} + \frac{B_{21}}{B_{11}B_{22}} & 0 \\ \frac{-B_{32}}{B_{22}B_{33}} + \frac{-2B_{22}B_{31}+2B_{21}B_{32}}{B_{11}B_{22}B_{33}} & -\frac{B_{32}}{B_{22}B_{33}} - \frac{-B_{22}B_{31}+B_{21}B_{32}}{B_{11}B_{22}B_{33}} & 0 \end{pmatrix} \in \mathbb{Z}^{3 \times 3}. \quad (6.4)$$

By inspection, it can be seen that equation 6.3 requires that $\frac{1}{B_{11}} \in \mathbb{Z}$. Because B_N is in Hermite normal form, this is only possible if $B_{11} = 1$. Rather than manually applying such logic successively to each element of B_N , we simply set $B_{11} = 1$ and then used Mathematica's Reduce function to simultaneously require that every element be integral. The result is that B_N must take one of the following forms:

$$B_N = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c_1 + 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 2 & 3 & 0 \\ 0 & 0 & c_1 + 1 \end{pmatrix}, \quad (6.5)$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 2c_1 + 2 & 2c_1 + 2 & 3c_1 + 3 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ c_1 + 1 & c_1 + 1 & 3c_1 + 3 \end{pmatrix}$$

where c_1 can be any non-negative integer. Now let us try to further restrict the four B_N families in equation 6.5 by imposing equation 3.11 on each one separately.

For the first matrix, we must have

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{c_1+1} \end{pmatrix} p_g \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c_1+1 \end{pmatrix} \in \mathbb{Z}^{3 \times 3} \quad (6.6)$$

for every $p_g \in P_G$. However, by inspection, we can see that every p_g commutes with the matrix so that the condition reduces to $p_g \in \mathbb{Z}^{3 \times 3}$, which does not further restrict B_N .

For the second matrix, the application of equation 3.11 to the five non-identity elements of P_G yields the following matrices:

$$\left\{ \begin{pmatrix} -2 & -3 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 3 & 0 \\ -1 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -2 & -3 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 3 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\}, \quad (6.7)$$

none of which contain fractions or depend on c_1 and thus do not further restrict B_N .

Application of equation 3.11 to the third and fourth matrices yields

$$\left\{ \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 2 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 2 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ -2 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & -1 \end{pmatrix} \right\} \in \mathbb{Z}^{3 \times 3} \quad (6.8)$$

and

$$\left\{ \begin{array}{l} \left(\begin{array}{ccc} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & 1 \end{array} \right), \left(\begin{array}{ccc} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 1 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{array} \right), \\ \left(\begin{array}{ccc} 1 & 0 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & -1 \end{array} \right), \left(\begin{array}{ccc} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & -1 \end{array} \right) \end{array} \right\} \in \mathbb{Z}^{3 \times 3}, \quad (6.9)$$

respectively. Again, both of these conditions are clearly true without further restricting the form of B_N .

For this particular G and P_N , imposing equation 3.11 does not restrict our solution any further. Hence, the four infinite families in equation 6.5 span all the possible normally supportive sublattices for the space group $P312$ (#149) and this particular normal cpg-subgroup P_N .

6.2 A Case with Bifurcation

Consider space group $Pmm2$ (#25), which has a point group $P_G = \{(x, y, z), (-x, -y, z), (-x, y, z), (x, -y, z)\}$ with the lattice coordinate representation

$$\left\{ \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{array} \right) \right\}. \quad (6.10)$$

P_G has the following five normal subgroups: $\{(x, y, z)\}$, $\{(x, y, z), (-x, -y, z)\}$, $\{(x, y, z), (-x, y, z)\}$, $\{(x, y, z), (x, -y, z)\}$, and $\{(x, y, z), (-x, -y, z), (-x, y, z), (x, -y, z)\}$. Let us consider the case of $P_N = m_y = \{(x, y, z), (x, -y, z)\}$.

When we impose equation 3.9 on the non-identity elements of P_N , Mathematica's Reduce

function yields the following eight B_N families:

$$\begin{aligned}
 B_N = & \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 2c_2 & 1+c_2+c_3 & 2+2c_2+2c_3 \end{pmatrix}, \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+2c_2 & 1+c_2+c_3 & 2+2c_2+2c_3 \end{pmatrix}, \\
 & \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 2c_2 & 0 & 2+2c_2+2c_3 \end{pmatrix}, \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 2c_2 & 0 & 1+2c_2+2c_3 \end{pmatrix}, \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+2c_2 & 0 & 2+2c_2+2c_3 \end{pmatrix}, \\
 & \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+2c_2 & 0 & 3+2c_2+2c_3 \end{pmatrix}, \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 2 & 0 \\ c_2 & 0 & 1+c_2+c_3 \end{pmatrix}, \begin{pmatrix} 1+c_1 & 0 & 0 \\ 1 & 2 & 0 \\ c_2 & 0 & 1+c_2+c_3 \end{pmatrix}
 \end{aligned} \tag{6.11}$$

where c_1 , c_2 , and c_3 can be any non-negative integers.

For the sake of brevity, we'll only consider the first B_N family in equation 6.11, to which the application of equation 3.11 yields the condition

$$\begin{pmatrix} \frac{1}{1+c_1} & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{c_2}{(1+c_1)(1+c_2+c_3)} & -\frac{1}{2} & \frac{1}{2+2c_2+2c_3} \end{pmatrix} p_g \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 2c_2 & 1+c_2+c_3 & 2+2c_2+2c_3 \end{pmatrix} \in \mathbb{Z}^{3 \times 3} \tag{6.12}$$

for each $p_g \in P_G$. Inserting each p_g then yields

$$\left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \frac{2c_2}{1+c_2+c_3} & 1 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{2c_2}{1+c_2+c_3} & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \right\} \in \mathbb{Z}^{3 \times 3} \tag{6.13}$$

which has only one nontrivial condition: $\frac{2c_2}{1+c_2+c_3} \in \mathbb{Z}$. There are two ways to satisfy this condition.

The first is to let $c_2 = 0$ and the second is to let $c_2 = c_3 + 1$. Applying these two replacements

separately effectively bifurcates the original B_N family into the following two families:

$$\begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1+c_2 & 2+2c_2 \end{pmatrix} \text{ and } \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 2+2c_2 & 2+2c_2 & 4+4c_2 \end{pmatrix} \quad (6.14)$$

where we have relabeled the old c_3 as the new c_2 for convenience, and where c_1 and c_2 can be any non-negative integers.

6.3 A Case with Extra Conditions

Consider space group $Imm2$ (#44) which has a point group $P_G = mm2_z$ whose point-group operators in the primitive setting are $\{(x, y, z), (y-z, x-z, -z), (x, x-z, x-y), (y-z, y, -x+y)\}$ with the lattice coordinate representation

$$\left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ -1 & -1 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & -1 \\ 1 & 1 & 1 \\ -1 & 0 & 0 \end{pmatrix} \right\}. \quad (6.15)$$

P_G has the following five normal subgroups: $\{(x, y, z)\}$, $\{(x, y, z), (y-z, x-z, -z)\}$, $\{(x, y, z), (x, x-z, x-y)\}$, $\{(x, y, z), (y-z, y, -x+y)\}$, and $\{(x, y, z), (y-z, x-z, -z), (x, x-z, x-y), (y-z, y, -x+y)\}$. Let us consider the case of $P_N = m_x = \{(x, y, z), (x, x-z, x-y)\}$.

When we impose equation 3.9 on the non-identity elements of P_N , Mathematica's Reduce function yields the following three B_N families:

$$B_N = \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ c_2 & 1 & 2+c_2+c_3 \end{pmatrix}, \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+c_2 & 1 & 2+c_2+c_3 \end{pmatrix} \quad (6.16)$$

where c_1 , c_2 , and c_3 can be any non-negative integers.

For this example, we'll only consider the third B_N family in equation 6.16, to which the application of equation 3.11 yields the condition

$$\begin{pmatrix} \frac{1}{1+c_1} & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{1+c_2}{(1+c_1)(2+c_2+c_3)} & -\frac{1}{2+c_2+c_3} & \frac{1}{2+c_2+c_3} \end{pmatrix} p_g \begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+c_2 & 1 & 2+c_2+c_3 \end{pmatrix} \in \mathbb{Z}^{3 \times 3} \quad (6.17)$$

for each $p_g \in P_G$. Inserting each p_g then yields

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -\frac{1+c_2}{1+c_1} & 0 & -\frac{2+c_2+c_3}{1+c_1} \\ c_1-c_2 & -1 & -2-c_2-c_3 \\ -\frac{(c_1-c_2)(2+c_1+c_2)}{(1+c_1)(2+c_2+c_3)} & 0 & \frac{1+c_2}{1+c_1} \end{pmatrix}, \quad (6.18)$$

$$\begin{pmatrix} 1 & 0 & 0 \\ c_1-c_2 & -1 & -2-c_2-c_3 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -\frac{1+c_2}{1+c_1} & 0 & -\frac{2+c_2+c_3}{1+c_1} \\ 0 & 1 & 0 \\ -\frac{(c_1-c_2)(2+c_1+c_2)}{(1+c_1)(2+c_2+c_3)} & 0 & \frac{1+c_2}{1+c_1} \end{pmatrix} \in \mathbb{Z}^{3 \times 3}.$$

This essentially has three nontrivial conditions: $\{d_1 = \frac{1+c_2}{1+c_1}, d_2 = \frac{2+c_2+c_3}{1+c_1}, d_3 = \frac{(c_1-c_2)(2+c_1+c_2)}{(1+c_1)(2+c_2+c_3)}\} \in \mathbb{Z}$. Using Mathematica's Reduce command under the assumption that all c and d variables are integers, we find that we can satisfy both of these conditions by bifurcating this B_N family into the following three cases.

For the first case, we let $d_1 = 1$ and $d_2 = 2$ by setting $c_2 = c_1$ and $c_3 = -2 - c_1 + 2 + 2c_1$. Making these substitutions will change d_3 to 0, which is trivially integral, and simplify B_N to

$$\begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+c_1 & 1 & 2+2c_1 \end{pmatrix} \quad (6.19)$$

where c_1 can be any non-negative integer.

For the second case, we let $d_1 = 1$ by setting $c_2 = c_1$ and $c_3 = -2 - c_1 + d_2 + c_1 d_2$. Making

these substitutions reduces d_3 to 0, which is trivially integral, and changes B_N to

$$\begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+c_1 & 1 & d_2+c_1d_2 \end{pmatrix}. \quad (6.20)$$

Because $d_2 = \frac{2+c_1+c_3}{1+c_1}$, where c_1 and c_3 can take on any non-negative integers, an appropriate value of c_3 will achieve any desired integer value of d_2 greater than 1 for any given non-negative integer value of c_1 . Thus, the range of d_2 is $d_2 \geq 2$. However, because we have already treated the $d_2 = 2$ case above, we will restrict the new B_N to the range $d_2 \geq 3$ in order to ensure that all B_N families are mutually disjoint. Finally, because it is convenient to define each variable in the B_N family over the range of non-negative integers, because d_2 does not appear in any extra conditions, and because the old c_2 variable is no longer being used, we define a new variable $c_2 = d_2 - 3 \geq 0$ and replace d_2 with $c_2 + 3$ within B_N to obtain

$$\begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ 1+c_1 & 1 & (1+c_1)(3+c_2) \end{pmatrix} \quad (6.21)$$

where c_1 and c_2 can be any non-negative integers.

For the third case, we let $c_2 = -1 + d_1 + c_1d_1$ and $c_3 = -1 - d_1 - c_1d_1 + d_2 + c_1d_2$, which reduces the d_3 condition to $\frac{1-d_1^2}{d_2} \in \mathbb{Z}$ and B_N to

$$\begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ d_1+c_1d_1 & 1 & d_2+c_1d_2 \end{pmatrix}. \quad (6.22)$$

Using similar logic to that applied in the previous case, and skipping the previously-treated $d_1 = 1$ scenario, our d -variable ranges are now $d_1 \geq 2$ and $d_2 \geq 1 + d_1$. For convenience, we replace d_1 with $2 + d_1$ and d_2 with $3 + d_1 + d_2$. Making these substitutions reduces the d_3 condition to

$\frac{3+4d_1+d_1^2}{3+d_1+d_2} \in \mathbb{Z}$ and B_N to

$$\begin{pmatrix} 1+c_1 & 0 & 0 \\ 0 & 1 & 0 \\ (1+c_1)(2+d_1) & 1 & (1+c_1)(3+d_1+d_2) \end{pmatrix}, \quad (6.23)$$

where c_1 , d_1 , and d_2 can be any non-negative integers that satisfy $\frac{3+4d_1+d_1^2}{3+d_1+d_2} \in \mathbb{Z}$.

6.4 A Very Messy Case

Consider space group *Amm2* (#38) which has a point group $P_G = mm2_z$ whose point-group operators in the primitive setting are $\{(x, y, z), (-x, z, y), (-x, y, z), (x, z, y)\}$ with the lattice coordinate representation

$$\left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right\}. \quad (6.24)$$

P_G has the following five normal subgroups: $\{(x, y, z)\}$, $\{(x, y, z), (-x, z, y)\}$, $\{(x, y, z), (-x, y, z)\}$, $\{(x, y, z), (x, z, y)\}$, and $\{(x, y, z), (-x, z, y), (-x, y, z), (x, z, y)\}$. Let us consider the case of $P_N = m_x = \{(x, y, z), (-x, y, z)\}$.

When we impose equation 3.9 on the non-identity elements of P_N , Mathematica's Reduce

function yields the following eight B_N families:

$$\begin{aligned}
 B_N = & \begin{pmatrix} 1 & 0 & 0 \\ 1+c_3 & 2+2c_3 & 0 \\ 1+c_1+c_2 & c_1 & 2+c_1+2c_2 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 1+c_3 & 2+2c_3 & 0 \\ c_1 & 2c_1 & 1+2c_1+c_2 \end{pmatrix}, \\
 & \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+c_3 & 0 \\ 0 & c_1 & 1+c_1+c_2 \end{pmatrix}, \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1+c_3 & 0 \\ 0 & c_1 & 1+c_1+c_2 \end{pmatrix}, \\
 & \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+c_2 & 0 \\ 1+c_1+c_3 & 2c_1 & 2+2c_1+2c_3 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+c_2 & 0 \\ 2+c_1+c_3 & 1+2c_1 & 4+2c_1+2c_3 \end{pmatrix}, \\
 & \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+c_2 & 0 \\ 1+c_1+c_3 & 1+2c_1 & 2+2c_1+2c_3 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+c_2 & 0 \\ 2+c_1+c_3 & 2+2c_1 & 4+2c_1+2c_3 \end{pmatrix}
 \end{aligned} \tag{6.25}$$

where c_1 , c_2 , and c_3 can be any non-negative integers.

For the sake of brevity, we'll only consider the first B_N family in equation 6.25, to which the application of equation 3.11 yields the condition

$$\begin{aligned}
 & \begin{pmatrix} 1 & 0 & 0 \\ -\frac{1+c_3}{2+2c_2} & \frac{1}{2+2c_2} & 0 \\ \frac{-2(1+c_2)^2+c_1(-1-2c_2+c_3)}{(2+2c_2)(2+c_1+2c_2)} & -\frac{c_1}{(2+2c_2)(2+c_1+2c_2)} & \frac{1}{2+c_1+2c_2} \end{pmatrix} p_g \\
 & * \begin{pmatrix} 1 & 0 & 0 \\ 1+c_3 & 2+2c_2 & 0 \\ 1+c_1+c_2 & c_1 & 2+c_1+2c_2 \end{pmatrix} \in \mathbb{Z}^{3 \times 3}
 \end{aligned} \tag{6.26}$$

for each $p_g \in P_G$. Inserting each p_g then yields

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ \frac{2+c_1+c_2+c_3}{2+2c_2} & \frac{c_1}{2+2c_2} & \frac{2+c_1+2c_2}{2+2c_2} \\ \frac{(2-c_1+2c_2)(2+c_1+c_2+c_3)}{(2+2c_2)(2+c_1+2c_2)} & \frac{2-c_1+2c_2}{2+2c_2} & -\frac{c_1}{2+2c_2} \end{pmatrix}, \quad (6.27)$$

$$\begin{pmatrix} -1 & 0 & 0 \\ \frac{1+c_3}{1+c_2} & 1 & 0 \\ \frac{2(1+c_2)^2+c_1(1+2c_2-c_3)}{(1+c_2)(2+c_1+2c_2)} & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ \frac{c_1+c_2-c_3}{2+2c_2} & \frac{c_1}{2+2c_2} & \frac{2+c_1+2c_2}{2+2c_2} \\ -\frac{c_1+c_2-c_3}{2+2c_2} & \frac{2-c_1+2c_2}{2+2c_2} & -\frac{c_1}{2+2c_2} \end{pmatrix}$$

which has five unique nontrivial conditions: $\{d_1 = \frac{c_1}{2+2c_3}, d_2 = \frac{2+c_1+2c_2}{2+2c_3}, d_3 = \frac{c_1+c_2-c_3}{2+2c_3}, d_4 = \frac{(c_1+c_2-c_3)(2+c_1+2c_3)}{(2+2c_3)(2+c_1+2c_2)}, d_5 = \frac{c_1^2-(2+2c_3)^2}{(2+2c_3)(2+c_1+2c_2)}\}$. Applying Mathematica's Reduce function under the assumption that all c and d variables are integers, we find that we can satisfy most of these conditions by breaking up B_N into the following seven cases.

For the first case, we set $c_1 = c_2 = c_3 = d_1 = d_3 = d_4 = 0$ and $d_2 = d_5 = 0$. This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \end{pmatrix}. \quad (6.28)$$

For the second case, we set $c_1 = c_3 = 0$ and $c_2 = -1 + d_2$ so that $d_1 = 0, d_3 = \frac{-1+d_2}{2}, d_4 = \frac{-1+d_2}{2d_2}$, and $d_5 = \frac{1}{d_2}$. This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ d_2 & 0 & 2d_2 \end{pmatrix} \quad (6.29)$$

where d_2 can be any integer greater than or equal to 2 that satisfies $\{\frac{-1+d_2}{2}, \frac{1}{d_2}\} \in \mathbb{Z}$. By inspection, it can be seen that no possible values of d_2 that will simultaneously satisfy all of these conditions and so this particular B_N family can be discarded.

For the third case, we set $c_1 = 0$ and $c_2 = c_3$ so that $d_1 = d_3 = d_4 = 0$ and $d_2 = d_5 = 1$. Then we define $c_1[\text{new}] = c_3[\text{old}] - 1$ so as to replace c_3 with $c_1 + 1$. This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ 2 + c_1 & 4 + 2c_1 & 0 \\ 2 + c_1 & 0 & 4 + 2c_1 \end{pmatrix} \quad (6.30)$$

where $c_1 \geq 0$.

For the fourth case, we set $c_1 = 0$ and $c_2 = -1 + d_2 + c_3 d_2$ so that $d_1 = 0$, $d_3 = \frac{-1+d_2}{2}$, $d_4 = \frac{-1+d_2}{2d_2}$, and $d_5 = \frac{1}{d_2}$. This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 + c_3 & 2 + 2c_3 & 0 \\ (1 + c_3)d_2 & 0 & (2 + 2c_3)d_2 \end{pmatrix} \quad (6.31)$$

where c_3 , and d_2 are integers that satisfy $c_3 d_2 > 0$, $d_2 \geq 2$, and $\{\frac{-1+d_2}{2}, \frac{1}{d_2}\} \in \mathbb{Z}$. By inspection, it can be seen that there are no solutions to these conditions and thus this B_N family can be discarded.

For the fifth case, we set $c_1 = 2d_1$ and $c_2 = c_3 = 0$ so that $d_2 = 1 + d_1$, $d_3 = d_4 = d_1$, and $d_5 = 1 - d_1$. Then we define $c_1[\text{new}] = d_1[\text{old}] - 1$ so as to replace d_1 with $c_1 + 1$. This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 3 + 2c_1 & 2 + 2c_1 & 4 + 2c_1 \end{pmatrix} \quad (6.32)$$

where $c_1 \geq 0$.

For the sixth case, we set $c_2 = c_3 = \frac{c_1 - 2d_1}{2d_1}$ so that $d_2 = 1 + d_1$, $d_3 = d_4 = d_1$, and $d_5 = 1 - d_1$.

This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ \frac{c_1}{2d_1} & \frac{c_1}{d_1} & 0 \\ c_1 + \frac{c_1}{2d_1} & c_1 & c_1 + \frac{c_1}{d_1} \end{pmatrix} \quad (6.33)$$

where c_1 and d_1 are any integers that satisfy $c_1 > 2d_1$, $d_1 \geq 1$, and $\frac{c_1}{2d_1} \in \mathbb{Z}$. Additional reduction is needed to bring this family into our prescribed form, which is

$$\begin{pmatrix} 1 & 0 & 0 \\ 2+c_1 & 2(2+c_1) & 0 \\ (2+c_1)(3+2c_2) & 2(2+c_1)(1+c_2) & 2(2+c_1)(2+c_2) \end{pmatrix} \quad (6.34)$$

where c_1 and c_2 can be any non-negative integers. However, we choose to skip the details here because we instead want to focus more attention on the seventh case.

For the seventh and final case (to which the remainder of this section will be devoted), we set $c_2 = \frac{-2d_1 - c_1 d_1 + c_1 d_2}{2d_1}$ and $c_3 = \frac{c_1 - 2d_1}{2d_1}$ so that $d_3 = \frac{-1+d_1+d_2}{2}$, $d_4 = \frac{(1+d_1)(-1+d_1+d_2)}{2d_2}$, and $d_5 = \frac{1-d_1^2}{d_2}$.

This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ \frac{c_1}{2d_1} & \frac{c_1}{d_1} & 0 \\ \frac{c_1(d_1+d_2)}{2d_1} & c_1 & \frac{c_1 d_2}{d_1} \end{pmatrix} \quad (6.35)$$

where c_1 , d_1 , and d_2 are any integers that satisfy $d_2 > 1+d_1$, $c_1 \geq 2d_1$, $d_1 \geq 1$, and $\left\{ \frac{(1+d_1)(-1+d_1+d_2)}{2d_1}, \frac{1-d_1^2}{d_2}, \frac{c_1}{2d_1}, \frac{-(2+c_1)d_1+c_1 d_2}{2d_1}, \frac{-1+d_1+d_2}{2} \right\} \in \mathbb{Z}$.

Here the quotients in B_N are undesirable because each element must be integral. To simplify B_N , we can replace d_1 with $\frac{c_1}{2g_1}$ which simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ d_1 & 2d_1 & 0 \\ d_1 d_2 + d_3 & 2d_3 & 2d_1 d_2 \end{pmatrix} \quad (6.36)$$

where, for convenience, g_1 and c_1 have been relabeled as d_1 and d_3 , respectively, and d_1 , d_2 , and d_3 can be any integers that satisfy $d_2 > 1 + \frac{d_3}{d_1}$, $d_3 \geq \frac{d_3}{d_1}$, $\frac{d_3}{d_1} \geq 1$, and $\left\{ \frac{(d_1+d_3)(d_1(-1+d_2)+d_3)}{4d_1^2 d_2}, \frac{d_1^2 - d_3^2}{d_1^2 d_2}, \frac{d_1(-1+d_2)+d_3}{2d_1}, \frac{d_3}{d_1} \right\} \in \mathbb{Z}$.

This B_N family is not ideal because the allowed ranges of values are dependent on other variables. To remedy this, we can again apply Mathematica's Reduce command which bifurcates

the family into three subcases. The first subcase has $d_1 = d_3 = 1$ and $d_2 \geq 3$. The second has $d_1 = 1$, $d_2 \geq 3$, $d_3 \geq 2$, and $d_2 > 1 + d_3$. The third has $d_1 \geq 2$, $d_2 \geq 3$, $d_1(-1 + d_2) > d_3$, and $d_3 \geq d_1$. Once again, for the sake of brevity, we will only explore the second subcase, which nicely illustrates some of the complexities encountered in producing Table A.1. For this subcase, B_N simplifies to

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ d_1 + d_2 & 2d_2 & 2d_1 \end{pmatrix}, \quad (6.37)$$

where for convenience, d_2 and d_3 have been relabeled as d_1 and d_2 , respectively, and d_1 and d_2 can be any integers that satisfy $d_1 \geq 3$, $d_2 \geq 2$, $d_1 > 1 + d_2$ and $\left\{ \frac{(1+d_2)(-1+d_1+d_2)}{2d_1}, \frac{-1+d_2^2}{d_1}, \frac{-1+d_1+d_2}{2} \right\} \in \mathbb{Z}$.

The extra condition $\frac{-1+d_1+d_2}{2} \in \mathbb{Z}$ can be eliminated if we define $k_1 = \frac{-1+d_1+d_2}{2}$ and then replace each occurrence of d_2 with $1 - d_1 + 2k_1$. This substitution simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1 + 2d_2 & 2 - 2d_1 + 4d_2 & 2d_1 \end{pmatrix}, \quad (6.38)$$

where k_1 has been relabeled $d_2[\text{new}]$ for convenience, and d_1 and d_2 can be any integers that satisfy $d_1 \geq 3$, $2d_2 \geq 1 + d_1$, $d_1 > 1 + d_2$ and $\frac{2(d_2+d_2^2)}{d_1} \in \mathbb{Z}$.

While the extra conditions are looking much cleaner, the ranges of the variables have grown significantly more convoluted. To remedy this, we again use Mathematica's Reduce command which replaces d_1 with $5 + 2d_1 + d_2$ and d_2 with $3 + d_1 + d_2$. This simplifies the B_N family to

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 7 + 2d_1 + 2d_2 & 4 + 2d_2 & 10 + 4d_1 + 2d_2 \end{pmatrix} \quad (6.39)$$

where d_1 and d_2 can be any non-negative integers that satisfy $\frac{2(2+3d_1+d_1^2)}{5+2d_1+d_2} \in \mathbb{Z}$.

We only followed the 2nd subcase of the 7th case bifurcated from the 1st B_N family from the application of equation 3.9. For $G = Amm2$ (ACC #15) and $P_N = m_x$, other threads were similarly complicated. Hence the extraordinary number of unique B_N families associated with this case, as seen in Table 5.1.

Chapter 7

Conclusions and Future Work

This thesis contains several key results. First, the cpg-normal subgroups for each crystallographic space group (i.e. normal subgroups of the point group of a space group) have been tabulated and the corresponding abstract quotient groups have been calculated. Second, we established two conditions that a sublattice T_N of crystallographic space group G must satisfy in order to support extensions with cpg-normal subgroup P_N that are normal subgroups of G . Third, an algorithm to find these normally supportive sublattices has been developed, along with Mathematica code that implements the algorithm. The algorithm first applies the simpler condition (inclusion, equation 3.9) to narrow the range of candidate sublattices, and then applies the more difficult condition (P_G -invariance, equation 3.11) to each sublattice that met the first condition. Fourth, the normally supportive sublattices only depend on the lattice centering type of the parent space group G and the cpg-normal subgroup P_N of the point group P_G of G ; we found that there are only 129 unique combinations of parent lattice centering and cpg-normal subgroup that need to be studied.

Fifth, we applied our code to determine and tabulate all of the normally supportive sublattices for each of the cpg-normal subgroups P_N of each of the 230 crystallographic space groups, excepting those cases for which P_N was the trivial subgroup 1 (these cases were too complicated with the present approach). Because space groups of the same arithmetic class have the same

cpg-normal subgroups, this analysis was only performed for the unique symmorphic space group from each arithmetic crystal class. Upon applying the inclusion condition (equation 3.9) to the 129 input scenarios, only 41 unique inclusion sublattices emerged. The P_G -invariance test (equation 3.11) required only the point-group operators of P_G and the unique inclusion sublattice associated with $P_N \subseteq P_G$. For a given arithmetic class and cpg-normal subgroup, the basis vectors of each normally-supportive sublattice are represented symbolically in Table A.1 by the columns of a B_N matrix in Hermite normal form. With considerable computer-guided algebraic manipulation, we were able to bring all but a handful of the B_N matrices into a standard form in which all variables have integer values, all variable ranges extend from zero to infinity, and no matrix elements contain quotients; however, some cases do include additional conditions on the variables (a quotient expression that is required to be integral). Four cases had slightly more complicated variable ranges. A matrix B_N containing symbolic variables actually represents an infinite family of sublattices, and in most cases, the complete set of normally-supportive sublattices could only be described using multiple B_N matrices that each represent multiple disjoint subfamilies. The most complicated case required 77 such subfamilies. A total of 1773 such B_N families are presented in Table A.1. The algebraic manipulation required to achieve the nice standard form was the most difficult aspect of this research. Of particular interest, a paper by Litvin and Kopský in 2000 claimed that cubic space groups will only have a finite number of normal subgroups [9]. Our results support this claim as there are no infinite B_N families corresponding to any of the cubic space groups (arithmetic crystal classes 59-73).

The ultimate goal of this research is to determine, in general, the types of topological defects that can be formed by the intersection of domain boundaries in crystals. During a crystal-crystal phase transition involving a loss of symmetry, domains of the low-symmetry phase form and eventually fill the volume of the crystal. The cosets of the child symmetry group H of the low-symmetry phase in the parent symmetry group G of the high-symmetry phase are acted upon by the symme-

tries of the quotient group $Q = G/N$, where N is the normal core of H in G . This action of Q on these cosets generates a coset graph, the topology of which appears to be relevant to the defect-topology problem.

Now that the normally supportive sublattices have been tabulated, the broader vision of understanding and possibly classifying the topologies of domain-interface defects will require additional work. The first step will be the group extension problem, or in other words combining P_N and T_N to obtain subgroups N of G (i.e. space groups in the same arithmetic crystal class as $T_N \times P_N$) [31]. The second step will be to enforce the normality condition $N \trianglelefteq G$ to obtain the csg-normal subgroups of G . Once the csg-normal subgroups of G are known, the third step will be to tabulate quotient groups $Q = G/N$ for each one. Fourth, a general strategy will be needed for generating the coset graph of a given Q and using it to deduce the defect-interface topologies that might result. By coset graph, we mean a complete colored digraph, wherein the vertices are the cosets of N in G , the arcs are ordered vertex pairs and the quotient group Q is an externally-defined vertex-transitive automorphism group whose action on the arcs assigns distinct colors to distinct arc orbits [32,33]. Figure 1.5 is an example of a coset graph with $G = P6_3/mmc$ (#194) and $N = P3c$ (#158).

Though difficult, the determination of normally-supportive sublattices was a necessary step in identifying and classifying the csg-normal subgroups of crystallographic space groups. The results should be useful in future work that aims to understand the topology of domain-intersection defects in crystals. After this work has been published, the code and relevant data files will be made available in a public Github repository.

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Appendix A

Normally Supportive Sublattices

Table A.1 A table of normally supportive sublattices of crystallographic space groups ordered by arithmetic crystal class and cpg-normal subgroup. The first column is the arithmetic class number and crystallographic space group representative. The second column is the cpg-normal subgroup P_N with a number and a name. The cpg-normal subgroup 1 in each case is omitted from this table for reasons explained in Chapter 3. The third column is the HNF matrix that represents a normally supportive sublattice laid out row by row. These matrices are numbered for convenience. The fourth column is an index (c#) which identifies additional conditions on the d parameters in B_N (rational polynomial functions that must have integer values) from Table A.2. An asterisk next to the c# denotes conditions that have no possible solutions. When no c# is provided, the variables can take on any non-negative integer values.

ACC	P_N	B_N matrix row by row	c#
$2 P\bar{1}$	$2 \bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
$2 P\bar{1}$	$2 \bar{1}$	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
$2 P\bar{1}$	$2 \bar{1}$	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
$3 P2$	$2 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
$3 P2$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
$3 P2$	$2 2_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
$3 P2$	$2 2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
$3 P2$	$2 2_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
$3 P2$	$2 2_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0, 1+c_1\}\}$	
$3 P2$	$2 2_z$	7 $\{\{1,0,0\}, \{0,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
$3 P2$	$2 2_z$	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
$3 P2$	$2 2_z$	9 $\{\{2,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
$3 P2$	$2 2_z$	10 $\{\{2,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
$3 P2$	$2 2_z$	11 $\{\{2,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
$4 C2$	$2 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
$4 C2$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
$4 C2$	$2 2_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
$4 C2$	$2 2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
$4 C2$	$2 2_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
$4 C2$	$2 2_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0, 1+c_1\}\}$	
$4 C2$	$2 2_z$	7 $\{\{1,0,0\}, \{0,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
$4 C2$	$2 2_z$	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
$4 C2$	$2 2_z$	9 $\{\{2,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
4 C2	$2 2_z$	10 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
4 C2	$2 2_z$	11 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
5 Pm	$2 m_z$	1 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{0, 0, 1\}\}$	
5 Pm	$2 m_z$	2 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{0, 0, 2\}\}$	
5 Pm	$2 m_z$	3 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{0, 1, 2\}\}$	
5 Pm	$2 m_z$	4 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{1, 0, 2\}\}$	
5 Pm	$2 m_z$	5 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{1, 1, 2\}\}$	
6 Cm	$2 m_z$	1 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{0, 0, 1\}\}$	
6 Cm	$2 m_z$	2 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{0, 0, 2\}\}$	
6 Cm	$2 m_z$	3 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{0, 1, 2\}\}$	
6 Cm	$2 m_z$	4 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{1, 0, 2\}\}$	
6 Cm	$2 m_z$	5 $\{\{1 + c_1, 0, 0\}, \{c_2, 1 + c_2 + c_3, 0\}, \{1, 1, 2\}\}$	
7 P2/m	$2 \bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
7 P2/m	$2 \bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
7 P2/m	$2 \bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
7 P2/m	$2 \bar{1}$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
7 P2/m	$2 \bar{1}$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
7 P2/m	$2 \bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
7 P2/m	$2 \bar{1}$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
7 P2/m	$2 \bar{1}$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
7 P2/m	$2 \bar{1}$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
7 P2/m	$2 \bar{1}$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
7 P2/m	$2 \bar{1}$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
7 P2/m	$2 \bar{1}$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
7 P2/m	$2 \bar{1}$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
7 P2/m	$2 \bar{1}$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
7 P2/m	$2 \bar{1}$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
7 P2/m	$2 \bar{1}$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
7 $P2/m$	3 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
7 $P2/m$	3 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
7 $P2/m$	3 2_z	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
7 $P2/m$	3 2_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
7 $P2/m$	3 2_z	5 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
7 $P2/m$	3 2_z	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0, 1+c_1\}\}$	
7 $P2/m$	3 2_z	7 $\{\{1,0,0\}, \{0,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
7 $P2/m$	3 2_z	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
7 $P2/m$	3 2_z	9 $\{\{2,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
7 $P2/m$	3 2_z	10 $\{\{2,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
7 $P2/m$	3 2_z	11 $\{\{2,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
7 $P2/m$	4 m_z	1 $\{\{1+c_1, 0, 0\}, \{c_2, 1+c_2+c_3, 0\}, \{0, 0, 1\}\}$	
7 $P2/m$	4 m_z	2 $\{\{1+c_1, 0, 0\}, \{c_2, 1+c_2+c_3, 0\}, \{0, 0, 2\}\}$	
7 $P2/m$	4 m_z	3 $\{\{1+c_1, 0, 0\}, \{c_2, 1+c_2+c_3, 0\}, \{0, 1, 2\}\}$	
7 $P2/m$	4 m_z	4 $\{\{1+c_1, 0, 0\}, \{c_2, 1+c_2+c_3, 0\}, \{1, 0, 2\}\}$	
7 $P2/m$	4 m_z	5 $\{\{1+c_1, 0, 0\}, \{c_2, 1+c_2+c_3, 0\}, \{1, 1, 2\}\}$	
7 $P2/m$	5 $2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
7 $P2/m$	5 $2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
7 $P2/m$	5 $2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
7 $P2/m$	5 $2/m_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
7 $P2/m$	5 $2/m_z$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
7 $P2/m$	5 $2/m_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
7 $P2/m$	5 $2/m_z$	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
7 $P2/m$	5 $2/m_z$	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
7 $P2/m$	5 $2/m_z$	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
7 $P2/m$	5 $2/m_z$	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
7 $P2/m$	5 $2/m_z$	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
7 $P2/m$	5 $2/m_z$	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
7 $P2/m$	$5 2/m_z$	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
7 $P2/m$	$5 2/m_z$	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
7 $P2/m$	$5 2/m_z$	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
7 $P2/m$	$5 2/m_z$	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
8 $C2/m$	$2 \bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
8 $C2/m$	$2 \bar{1}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
8 $C2/m$	$2 \bar{1}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
8 $C2/m$	$2 \bar{1}$	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
8 $C2/m$	$2 \bar{1}$	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
8 $C2/m$	$2 \bar{1}$	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
8 $C2/m$	$2 \bar{1}$	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
8 $C2/m$	$2 \bar{1}$	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
8 $C2/m$	$2 \bar{1}$	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
8 $C2/m$	$3 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
8 $C2/m$	$3 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
8 $C2/m$	$3 2_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
8 $C2/m$	$3 2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
8 $C2/m$	$3 2_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
8 $C2/m$	$3 2_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0, 1+c_1\}\}$	
8 $C2/m$	$3 2_z$	7 $\{\{1,0,0\}, \{0,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
8 $C2/m$	$3 2_z$	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
8 $C2/m$	$3 2_z$	9 $\{\{2,0,0\}, \{0,1,0\}, \{0,1+c_1,2+2c_1\}\}$	
8 $C2/m$	$3 2_z$	10 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
8 $C2/m$	$3 2_z$	11 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
8 $C2/m$	$4 m_z$	1 $\{\{1+c_1,0,0\}, \{c_2,1+c_2+c_3,0\}, \{0,0,1\}\}$	
8 $C2/m$	$4 m_z$	2 $\{\{1+c_1,0,0\}, \{c_2,1+c_2+c_3,0\}, \{0,0,2\}\}$	
8 $C2/m$	$4 m_z$	3 $\{\{1+c_1,0,0\}, \{c_2,1+c_2+c_3,0\}, \{0,1,2\}\}$	
8 $C2/m$	$4 m_z$	4 $\{\{1+c_1,0,0\}, \{c_2,1+c_2+c_3,0\}, \{1,0,2\}\}$	
8 $C2/m$	$4 m_z$	5 $\{\{1+c_1,0,0\}, \{c_2,1+c_2+c_3,0\}, \{1,1,2\}\}$	
8 $C2/m$	$5 2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
8 $C2/m$	$5 2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
8 $C2/m$	$5 2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
8 $C2/m$	$5 2/m_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
8 $C2/m$	$5 2/m_z$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
8 $C2/m$	$5 2/m_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
8 $C2/m$	$5 2/m_z$	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
8 $C2/m$	$5 2/m_z$	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
8 $C2/m$	$5 2/m_z$	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
8 $C2/m$	$5 2/m_z$	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
8 $C2/m$	$5 2/m_z$	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
8 $C2/m$	$5 2/m_z$	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
8 $C2/m$	$5 2/m_z$	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
8 $C2/m$	$5 2/m_z$	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
8 $C2/m$	$5 2/m_z$	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
8 $C2/m$	$5 2/m_z$	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
9 $P222$	$2 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,1+c_1,2+2c_1\}\}$	
9 $P222$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,0,2+2c_1\}\}$	
9 $P222$	$2 2_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,1+c_1,2+2c_1\}\}$	
9 $P222$	$2 2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
9 P222	2 2 _z	5 {{1,0,0},{1,2,0},{1+c ₁ ,0,2+2c ₁ }}	
9 P222	2 2 _z	6 {{1,0,0},{1,2,0},{0,0,1+c ₁ }}	
9 P222	2 2 _z	7 {{1,0,0},{0,2,0},{1+c ₁ ,0,2+2c ₁ }}	
9 P222	2 2 _z	8 {{1,0,0},{0,2,0},{0,0,1+c ₁ }}	
9 P222	2 2 _z	9 {{2,0,0},{0,1,0},{0,1+c ₁ ,2+2c ₁ }}	
9 P222	2 2 _z	10 {{2,0,0},{0,1,0},{0,0,1+c ₁ }}	
9 P222	2 2 _z	11 {{2,0,0},{0,2,0},{0,0,1+c ₁ }}	
9 P222	3 2 _y	1 {{1,0,0},{1+c ₁ ,2+2c ₁ ,0},{0,0,1}}	
9 P222	3 2 _y	2 {{1,0,0},{0,1+c ₁ ,0},{0,0,1}}	
9 P222	3 2 _y	3 {{1,0,0},{1+c ₁ ,2+2c ₁ ,0},{1,0,2}}	
9 P222	3 2 _y	4 {{1,0,0},{1+c ₁ ,2+2c ₁ ,0},{0,0,2}}	
9 P222	3 2 _y	5 {{1,0,0},{0,1+c ₁ ,0},{1,0,2}}	
9 P222	3 2 _y	6 {{1,0,0},{0,1+c ₁ ,0},{1,1,2}}	
9 P222	3 2 _y	7 {{1,0,0},{0,1+c ₁ ,0},{0,0,2}}	
9 P222	3 2 _y	8 {{1,0,0},{0,1+c ₁ ,0},{0,1,2}}	
9 P222	3 2 _y	9 {{2,0,0},{0,1+c ₁ ,0},{0,0,1}}	
9 P222	3 2 _y	10 {{2,0,0},{0,1+c ₁ ,0},{0,0,2}}	
9 P222	3 2 _y	11 {{2,0,0},{0,1+c ₁ ,0},{0,1,2}}	
9 P222	4 2 _x	1 {{1+c ₁ ,0,0},{0,1,0},{0,0,1}}	
9 P222	4 2 _x	2 {{1+c ₁ ,0,0},{0,1,0},{0,1,2}}	
9 P222	4 2 _x	3 {{1+c ₁ ,0,0},{0,1,0},{1,1,2}}	
9 P222	4 2 _x	4 {{1+c ₁ ,0,0},{0,1,0},{0,0,2}}	
9 P222	4 2 _x	5 {{1+c ₁ ,0,0},{0,1,0},{1,0,2}}	
9 P222	4 2 _x	6 {{1+c ₁ ,0,0},{0,2,0},{0,0,1}}	
9 P222	4 2 _x	7 {{1+c ₁ ,0,0},{1,2,0},{0,0,1}}	
9 P222	4 2 _x	8 {{1+c ₁ ,0,0},{0,2,0},{0,0,2}}	
9 P222	4 2 _x	9 {{1+c ₁ ,0,0},{0,2,0},{1,0,2}}	
9 P222	4 2 _x	10 {{1+c ₁ ,0,0},{1,2,0},{0,0,2}}	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
9 P222	4 2_x	11 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
9 P222	5 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
9 P222	5 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
9 P222	5 222	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
9 P222	5 222	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
9 P222	5 222	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
9 P222	5 222	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
9 P222	5 222	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
9 P222	5 222	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
9 P222	5 222	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
9 P222	5 222	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
9 P222	5 222	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
9 P222	5 222	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
9 P222	5 222	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
9 P222	5 222	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
9 P222	5 222	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
9 P222	5 222	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
10 C222	2 2_z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
10 C222	2 2_z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
10 C222	2 2_z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
10 C222	2 2_z	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
10 C222	2 2_z	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
10 C222	3 2_y	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
10 C222	3 2_y	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
10 C222	3 2_y	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 1, 2\}\}$	
10 C222	4 2_x	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
10 C222	4 2_x	2 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 1\}\}$	
10 C222	4 2_x	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
10 C222	4 2_x	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
10 C222	4 2_x	5 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,0,2\}\}$	
10 C222	4 2_x	6 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,1,2\}\}$	
10 C222	5 222	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
10 C222	5 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
10 C222	5 222	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
10 C222	5 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
10 C222	5 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
11 F222	2 2_z	1 $\{\{1,0,0\}, \{c_1,1+c_1,0\}, \{1,0,2\}\}$	
11 F222	2 2_z	2 $\{\{1,0,0\}, \{c_1,1+c_1,0\}, \{0,1,2\}\}$	
11 F222	2 2_z	3 $\{\{1,0,0\}, \{c_1,1+c_1,0\}, \{0,0,1\}\}$	
11 F222	3 2_y	1 $\{\{1,0,0\}, \{1,2,0\}, \{c_1,0,1+c_1\}\}$	
11 F222	3 2_y	2 $\{\{1,0,0\}, \{0,1,0\}, \{c_1,1+c_1,2+2c_1\}\}$	
11 F222	3 2_y	3 $\{\{1,0,0\}, \{0,1,0\}, \{c_1,0,1+c_1\}\}$	
11 F222	4 2_x	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
11 F222	4 2_x	2 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, c_1, 2+c_1\}\}$	
11 F222	4 2_x	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, c_1, 1+c_1\}\}$	
11 F222	4 2_x	4 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, c_1, 2+2c_1\}\}$	
11 F222	5 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
11 F222	5 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
11 F222	5 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
11 F222	5 222	4 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
11 F222	5 222	5 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
12 I222	2 2_z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
12 I222	2 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
12 I222	2 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
12 I222	2 2_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
12 I222	2 2_z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
12 I222	3 2_y	1 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
12 I222	3 2_y	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
12 I222	3 2_y	3 $\{\{1,0,0\}, \{0,2,0\}, \{3+2c_1, 2, 2(2+c_1)\}\}$	
12 I222	3 2_y	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+4c_1, 3+2c_1, 4(1+c_1)\}\}$	
12 I222	3 2_y	5 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1, 2+c_1\}\}$	
12 I222	4 2_x	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
12 I222	4 2_x	2 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+4c_1, 4(1+c_1)\}\}$	
12 I222	4 2_x	3 $\{\{1,0,0\}, \{0,1,0\}, \{1, 1+c_1, 2+c_1\}\}$	
12 I222	4 2_x	4 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
12 I222	4 2_x	5 $\{\{2,0,0\}, \{0,1,0\}, \{2, 3+2c_1, 2(2+c_1)\}\}$	
12 I222	5 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
12 I222	5 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
12 I222	5 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
12 I222	5 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
12 I222	5 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
12 I222	5 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
13 Pmm2	2 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
13 Pmm2	2 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
13 Pmm2	2 2_z	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
13 Pmm2	2 2_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
13 Pmm2	2 2_z	5 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
13 Pmm2	2 2_z	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0, 1+c_1\}\}$	
13 Pmm2	2 2_z	7 $\{\{1,0,0\}, \{0,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
13 Pmm2	2 2_z	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
13 Pmm2	2 2_z	9 $\{\{2,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
13 Pmm2	2 2_z	10 $\{\{2,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
13 Pmm2	2 2_z	11 $\{\{2,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
13 Pmm2	3 m_x	1 $\{\{1,0,0\}, \{1+c_1, 2(1+c_1), 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
13 $Pmm2$	$3 m_x$	2 $\{\{1,0,0\}, \{1+c_1, 2(1+c_1), 0\}, \{0,0, 1+c_2\}\}$	
13 $Pmm2$	$3 m_x$	3 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{0,0, 1+c_2\}\}$	
13 $Pmm2$	$3 m_x$	4 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{0, 1+c_2, 2(1+c_2)\}\}$	
13 $Pmm2$	$3 m_x$	5 $\{\{2,0,0\}, \{0, 1+c_1, 0\}, \{0,0, 1+c_2\}\}$	
13 $Pmm2$	$3 m_x$	6 $\{\{2,0,0\}, \{0, 1+c_1, 0\}, \{0, 1+c_2, 2(1+c_2)\}\}$	
13 $Pmm2$	$3 m_x$	7 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	
13 $Pmm2$	$3 m_x$	8 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{2(1+c_2), 2(1+c_2), 4(1+c_2)\}\}$	
13 $Pmm2$	$3 m_x$	9 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{3+2c_2, 3+2c_2, 6+4c_2\}\}$	
13 $Pmm2$	$3 m_x$	10 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{1+2c_2, 1+2c_2, 2+4c_2\}\}$	
13 $Pmm2$	$3 m_x$	11 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{2(1+c_2), 2(1+c_2), 4(1+c_2)\}\}$	
13 $Pmm2$	$4 m_y$	1 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1+c_2, 2(1+c_2)\}\}$	
13 $Pmm2$	$4 m_y$	2 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{2(1+c_2), 2(1+c_2), 4(1+c_2)\}\}$	
13 $Pmm2$	$4 m_y$	3 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{1+2c_2, 1+2c_2, 2+4c_2\}\}$	
13 $Pmm2$	$4 m_y$	4 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2(1+c_2)\}\}$	
13 $Pmm2$	$4 m_y$	5 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{2(1+c_2), 0, 4(1+c_2)\}\}$	
13 $Pmm2$	$4 m_y$	6 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1+2c_2\}\}$	
13 $Pmm2$	$4 m_y$	7 $\{\{1+c_1, 0, 0\}, \{0, 1, 0\}, \{1+2c_2, 0, 2+4c_2\}\}$	
13 $Pmm2$	$4 m_y$	8 $\{\{1+c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1+c_2\}\}$	
13 $Pmm2$	$4 m_y$	9 $\{\{1+c_1, 0, 0\}, \{0, 2, 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	
13 $Pmm2$	$4 m_y$	10 $\{\{1+c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1+c_2\}\}$	
13 $Pmm2$	$4 m_y$	11 $\{\{1+c_1, 0, 0\}, \{1, 2, 0\}, \{1+c_2, 0, 2(1+c_2)\}\}$	
13 $Pmm2$	$5 mm2_z$	1 $\{\{1,0,0\}, \{0, 1, 0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	2 $\{\{1,0,0\}, \{0, 1, 0\}, \{1+c_1, 0, 2+2c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	3 $\{\{1,0,0\}, \{0, 1, 0\}, \{0, 1+c_1, 2+2c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	4 $\{\{1,0,0\}, \{0, 1, 0\}, \{0, 0, 1+c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	5 $\{\{1,0,0\}, \{1, 2, 0\}, \{1+c_1, 0, 2+2c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	6 $\{\{1,0,0\}, \{1, 2, 0\}, \{0, 0, 1+c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	7 $\{\{1,0,0\}, \{0, 2, 0\}, \{1+c_1, 0, 2+2c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
13 $Pmm2$	$5 mm2_z$	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	9 $\{\{2,0,0\}, \{0,1,0\}, \{0,1+c_1,2+2c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	10 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
13 $Pmm2$	$5 mm2_z$	11 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
14 $Cmm2$	$2 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,1+c_1,2+2c_1\}\}$	
14 $Cmm2$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
14 $Cmm2$	$2 2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1,0,2+2c_1\}\}$	
14 $Cmm2$	$2 2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
14 $Cmm2$	$2 2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
14 $Cmm2$	$3 m_x$	1 $\{\{1,0,0\}, \{c_1,1+c_1,0\}, \{0,0,1+c_2\}\}$	
14 $Cmm2$	$3 m_x$	2 $\{\{1,0,0\}, \{c_1,1+c_1,0\}, \{1+c_2,1+c_2,2(1+c_2)\}\}$	
14 $Cmm2$	$4 m_y$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
14 $Cmm2$	$4 m_y$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,1+c_1,2(1+c_1)\}\}$	
14 $Cmm2$	$4 m_y$	3 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,0,1+c_2\}\}$	
14 $Cmm2$	$4 m_y$	4 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,1+c_2,2(1+c_2)\}\}$	
14 $Cmm2$	$5 mm2_z$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
14 $Cmm2$	$5 mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,1+c_1,2+2c_1\}\}$	
14 $Cmm2$	$5 mm2_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
15 $Amm2$	$2 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,1+2c_1,2+2c_1\}\}$	
15 $Amm2$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,c_1,1+c_1\}\}$	
15 $Amm2$	$2 2_z$	3 $\{\{2,0,0\}, \{0,1,0\}, \{0,c_1,1+c_1\}\}$	
15 $Amm2$	$3 m_x$	1 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
15 $Amm2$	$3 m_x$	2 $\{\{1,0,0\}, \{1,2,0\}, \{3+2c_1,2(1+c_1),2(2+c_1)\}\}$	
15 $Amm2$	$3 m_x$	3 $\{\{1,0,0\}, \{1,2,0\}, \{5+2c_1,2,4(2+c_1)\}\}$	
15 $Amm2$	$3 m_x$	4 $\{\{1,0,0\}, \{2+c_1,2(2+c_1),0\}, \{2+c_1,0,2(2+c_1)\}\}$	
15 $Amm2$	$3 m_x$	5 $\{\{1,0,0\}, \{2+c_1,2(2+c_1),0\},$ $\{(2+c_1)(3+2c_2),2(2+c_1)(1+c_2),2(2+c_1)(2+c_2)\}\}$	
15 $Amm2$	$3 m_x$	6 $\{\{1,0,0\}, \{1,2,0\}, \{7+2d_1+2d_2,2(2+d_2),2(5+2d_1+d_2)\}\}$	21

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
15 Amm2	$3 m_x$	7 $\{\{1,0,0\}, \{2+c_1, 2(2+c_1), 0\},$ $\{(2+c_1)(5+2d_1+2d_2), 2(2+c_1)(1+d_2), 2(2+c_1)(4+2d_1+d_2)\}\}$	57
15 Amm2	$3 m_x$	8 $\{\{1,0,0\}, \{2,4,0\}, \{2,4,8\}\}$	
15 Amm2	$3 m_x$	9 $\{\{1,0,0\}, \{1,2,0\}, \{1,2, 2(2+c_1)\}\}$	
15 Amm2	$3 m_x$	10 $\{\{1,0,0\}, \{3+c_1, 2(3+c_1), 0\}, \{3+c_1, 2(3+c_1), 4(3+c_1)\}\}$	
15 Amm2	$3 m_x$	11 $\{\{1,0,0\}, \{1,2,0\}, \{3+2d_1, 6+4d_1, 2(4+2d_1+d_2)\}\}$	20
15 Amm2	$3 m_x$	12 $\{\{1,0,0\}, \{2,4,0\}, \{2+4d_1, 4+8d_1, 4(3+2d_1+d_2)\}\}$	19
15 Amm2	$3 m_x$	13 $\{\{1,0,0\}, \{2,4,0\}, \{6+4d_1, 12+8d_1, 4(4+2d_1+d_2)\}\}$	20
15 Amm2	$3 m_x$	14 $\{\{1,0,0\}, \{3+c_1, 2(3+c_1), 0\},$ $\{(3+c_1)(1+2d_1), (3+c_1)(2+4d_1), 2(3+c_1)(3+2d_1+d_2)\}\}$	54
15 Amm2	$3 m_x$	15 $\{\{1,0,0\}, \{3+c_1, 2(3+c_1), 0\},$ $\{(3+c_1)(3+2d_1), 2(3+c_1)(3+2d_1), 2(3+c_1)(4+2d_1+d_2)\}\}$	56
15 Amm2	$3 m_x$	16 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
15 Amm2	$3 m_x$	17 $\{\{1,0,0\}, \{0,2,0\}, \{0,2,6\}\}$	
15 Amm2	$3 m_x$	18 $\{\{1,0,0\}, \{0,1,0\}, \{0,1, 3+c_1\}\}$	
15 Amm2	$3 m_x$	19 $\{\{1,0,0\}, \{0,1,0\}, \{0,1+c_1, 2+c_1\}\}$	
15 Amm2	$3 m_x$	20 $\{\{1,0,0\}, \{0,2+c_1, 0\}, \{0,0, 2+c_1\}\}$	
15 Amm2	$3 m_x$	21 $\{\{1,0,0\}, \{0,3+c_1, 0\}, \{0,3+c_1, 3(3+c_1)\}\}$	
15 Amm2	$3 m_x$	22 $\{\{1,0,0\}, \{0,2+c_1, 0\}, \{0, (2+c_1)(1+c_2), (2+c_1)(2+c_2)\}\}$	
15 Amm2	$3 m_x$	23 $\{\{1,0,0\}, \{0,1,0\}, \{0,2+d_1, 4+d_1+d_2\}\}$	14
15 Amm2	$3 m_x$	24 $\{\{1,0,0\}, \{0,2,0\}, \{0,2(1+d_1), 2(4+d_1+d_2)\}\}$	12
15 Amm2	$3 m_x$	25 $\{\{1,0,0\}, \{0,2,0\}, \{0,2(2+d_1), 2(4+d_1+d_2)\}\}$	14
15 Amm2	$3 m_x$	26 $\{\{1,0,0\}, \{0,3+c_1, 0\}, \{0, (3+c_1)(1+d_1), (3+c_1)(4+d_1+d_2)\}\}$	45
15 Amm2	$3 m_x$	27 $\{\{1,0,0\}, \{0,3+c_1, 0\}, \{0, (3+c_1)(2+d_1), (3+c_1)(4+d_1+d_2)\}\}$	47
15 Amm2	$3 m_x$	28 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
15 Amm2	$3 m_x$	29 $\{\{2,0,0\}, \{0,2,0\}, \{0,2,6\}\}$	
15 Amm2	$3 m_x$	30 $\{\{2,0,0\}, \{0,1,0\}, \{0,1, 3+c_1\}\}$	
15 Amm2	$3 m_x$	31 $\{\{2,0,0\}, \{0,1,0\}, \{0,1+c_1, 2+c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
15 Amm2	$3 m_x$	32 $\{\{2, 0, 0\}, \{0, 2 + c_1, 0\}, \{0, 0, 2 + c_1\}\}$	
15 Amm2	$3 m_x$	33 $\{\{2, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, 3 + c_1, 3(3 + c_1)\}\}$	
15 Amm2	$3 m_x$	34 $\{\{2, 0, 0\}, \{0, 2 + c_1, 0\}, \{0, (2 + c_1)(1 + c_2), (2 + c_1)(2 + c_2)\}\}$	
15 Amm2	$3 m_x$	35 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 2 + d_1, 4 + d_1 + d_2\}\}$	14
15 Amm2	$3 m_x$	36 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 2(1 + d_1), 2(4 + d_1 + d_2)\}\}$	12
15 Amm2	$3 m_x$	37 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 2(2 + d_1), 2(4 + d_1 + d_2)\}\}$	14
15 Amm2	$3 m_x$	38 $\{\{2, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, (3 + c_1)(1 + d_1), (3 + c_1)(4 + d_1 + d_2)\}\}$	45
15 Amm2	$3 m_x$	39 $\{\{2, 0, 0\}, \{0, 3 + c_1, 0\}, \{0, (3 + c_1)(2 + d_1), (3 + c_1)(4 + d_1 + d_2)\}\}$	47
15 Amm2	$3 m_x$	40 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2, 2, 4\}\}$	
15 Amm2	$3 m_x$	41 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{4, 2, 8\}\}$	
15 Amm2	$3 m_x$	42 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{4(1 + c_1), 6(1 + c_1), 8(1 + c_1)\}\}$	
15 Amm2	$3 m_x$	43 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{2(2 + c_1), 2(2 + c_1), 4(2 + c_1)\}\}$	
15 Amm2	$3 m_x$	44 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{4(2 + c_1), 2(2 + c_1), 8(2 + c_1)\}\}$	
15 Amm2	$3 m_x$	45 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(3 + c_2), 2(1 + c_1)(5 + 2c_2), 4(1 + c_1)(3 + c_2)\}\}$	
15 Amm2	$3 m_x$	46 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(4 + d_1 + 2d_2), 6 + 4d_1 + 4d_2, 4(4 + d_1 + 2d_2)\}\}$	26
15 Amm2	$3 m_x$	47 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(4 + d_1 + 2d_2), 10 + 4d_1 + 4d_2, 4(4 + d_1 + 2d_2)\}\}$	27
15 Amm2	$3 m_x$	48 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(3 + d_1 + 2d_2), 2 + 4d_1 + 4d_2, 4(3 + d_1 + 2d_2)\}\}$	29
15 Amm2	$3 m_x$	49 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{2(3 + d_1 + 2d_2), 6 + 4d_1 + 4d_2, 4(3 + d_1 + 2d_2)\}\}$	28
15 Amm2	$3 m_x$	50 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\},$ $\{2(2 + c_1)(3 + d_1 + d_2), 2(2 + c_1)(1 + 2d_1), 4(2 + c_1)(3 + d_1 + d_2)\}\}$	37
15 Amm2	$3 m_x$	51 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\},$ $\{2(2 + c_1)(3 + d_1 + d_2), 2(2 + c_1)(3 + 2d_1), 4(2 + c_1)(3 + d_1 + d_2)\}\}$	40
15 Amm2	$3 m_x$	52 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{4(2 + c_1), 6(2 + c_1), 8(2 + c_1)\}\}$	
15 Amm2	$3 m_x$	53 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{2 + 4c_1, 1 + 2c_1, 4 + 8c_1\}\}$	
15 Amm2	$3 m_x$	54 $\{\{1, 0, 0\}, \{0, 3 + 2c_1, 0\}, \{3 + 2c_1, 3 + 2c_1, 6 + 4c_1\}\}$	
15 Amm2	$3 m_x$	55 $\{\{1, 0, 0\}, \{0, 3 + 2c_1, 0\}, \{9 + 6c_1, 5(3 + 2c_1), 6(3 + 2c_1)\}\}$	
15 Amm2	$3 m_x$	56 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{(1 + 2c_1)(3 + c_2), 1 + 2c_1, 2(1 + 2c_1)(3 + c_2)\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
15 Amm2	$3 m_x$	57 $\{\{1, 0, 0\}, \{0, 3 + 2c_1, 0\},$ $\{(3 + 2c_1)(4 + c_2), (3 + 2c_1)(7 + 2c_2), 2(3 + 2c_1)(4 + c_2)\}\}$	
15 Amm2	$3 m_x$	58 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{4 + d_1 + d_2, 3 + 2d_1, 2(4 + d_1 + d_2)\}\}$	13
15 Amm2	$3 m_x$	59 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{4 + d_1 + d_2, 5 + 2d_1, 2(4 + d_1 + d_2)\}\}$	15
15 Amm2	$3 m_x$	60 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(3 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	46
15 Amm2	$3 m_x$	61 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(5 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	48
15 Amm2	$3 m_x$	62 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{2, 3, 4\}\}$	
15 Amm2	$3 m_x$	63 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{4(1 + c_1), 6(1 + c_1), 8(1 + c_1)\}\}$	
15 Amm2	$3 m_x$	64 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{1 + 2c_1, 1 + 2c_1, 2 + 4c_1\}\}$	
15 Amm2	$3 m_x$	65 $\{\{1, 0, 0\}, \{0, 1 + 2c_1, 0\}, \{(1 + 2c_1)(2 + c_2), 1 + 2c_1, 2(1 + 2c_1)(2 + c_2)\}\}$	
15 Amm2	$3 m_x$	66 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + d_1 + d_2, 3 + 2d_1, 2(3 + d_1 + d_2)\}\}$	8
15 Amm2	$3 m_x$	67 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3 + d_1 + d_2, 5 + 2d_1, 2(3 + d_1 + d_2)\}\}$	11
15 Amm2	$3 m_x$	68 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(3 + d_1 + d_2), 2(1 + c_1)(3 + 2d_1), 4(1 + c_1)(3 + d_1 + d_2)\}\}$	41
15 Amm2	$3 m_x$	69 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(3 + d_1 + d_2), 2(1 + c_1)(5 + 2d_1), 4(1 + c_1)(3 + d_1 + d_2)\}\}$	44
15 Amm2	$3 m_x$	70 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{4, 6, 8\}\}$	
15 Amm2	$3 m_x$	71 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{2(1 + c_1), 2(1 + c_1), 4(1 + c_1)\}\}$	
15 Amm2	$3 m_x$	72 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\}, \{6(1 + c_1), 10(1 + c_1), 12(1 + c_1)\}\}$	
15 Amm2	$3 m_x$	73 $\{\{1, 0, 0\}, \{0, 2(2 + c_1), 0\}, \{4(2 + c_1), 6(2 + c_1), 8(2 + c_1)\}\}$	
15 Amm2	$3 m_x$	74 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(2 + c_2), 2(1 + c_1), 4(1 + c_1)(2 + c_2)\}\}$	
15 Amm2	$3 m_x$	75 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(4 + c_2), 2(1 + c_1)(7 + 2c_2), 4(1 + c_1)(4 + c_2)\}\}$	
15 Amm2	$3 m_x$	76 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(3 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	46

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
15 <i>Amm2</i>	3 m_x	77 $\{\{1, 0, 0\}, \{0, 2(1 + c_1), 0\},$ $\{2(1 + c_1)(4 + d_1 + d_2), 2(1 + c_1)(5 + 2d_1), 4(1 + c_1)(4 + d_1 + d_2)\}\}$	48
15 <i>Amm2</i>	4 m_y	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, c_2, 1 + c_2\}\}$	
15 <i>Amm2</i>	4 m_y	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + c_2, 1 + 2c_2, 2(1 + c_2)\}\}$	
15 <i>Amm2</i>	5 $mm2_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + 2c_1, 2 + 2c_1\}\}$	
15 <i>Amm2</i>	5 $mm2_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
15 <i>Amm2</i>	5 $mm2_z$	3 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, c_1, 1 + c_1\}\}$	
16 <i>Fmm2</i>	2 2_z	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2\}\}$	
16 <i>Fmm2</i>	2 2_z	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 1, 2\}\}$	
16 <i>Fmm2</i>	2 2_z	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
16 <i>Fmm2</i>	3 m_x	1 $\{\{1, 0, 0\}, \{c_2, 1 + c_2, 0\}, \{c_1, 0, 1 + c_1\}\}$	
16 <i>Fmm2</i>	3 m_x	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{c_2, 1 + c_2, 2(1 + c_2)\}\}$	
16 <i>Fmm2</i>	4 m_y	1 $\{\{1, 0, 0\}, \{(1 + c_1)c_2, 1 + c_2 + c_1c_2, 0\}, \{0, c_1, 1 + c_1\}\}$	
16 <i>Fmm2</i>	4 m_y	2 $\{\{1, 0, 0\}, \{(1 + c_1)(1 + 2c_2), 2 + c_1 + 2c_2 + 2c_1c_2, 0\},$ $\{0, 1 + 2c_1, 2(1 + c_1)\}\}$	
16 <i>Fmm2</i>	4 m_y	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 0, 2(1 + c_1)\}\}$	
16 <i>Fmm2</i>	4 m_y	4 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_1 + 2c_2)\}\}$	
16 <i>Fmm2</i>	4 m_y	5 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{3 + 2c_2, 2(1 + c_2), 2(3 + c_1 + 2c_2)\}\}$	
16 <i>Fmm2</i>	4 m_y	6 $\{\{1, 0, 0\}, \{1 + 2c_3 + 2c_1(1 + c_2 + c_3), 2(1 + c_3 + c_1(1 + c_2 + c_3)), 0\},$ $\{1 + 2c_2, 2c_2, 2(1 + c_2 + c_3)\}\}$	
16 <i>Fmm2</i>	4 m_y	7 $\{\{1, 0, 0\}, \{2 + c_2 + 3c_3 + 2c_1(1 + c_2 + c_3),$ $3 + c_2 + 3c_3 + 2c_1(1 + c_2 + c_3), 0\}, \{1 + 2c_2, 2c_2, 2(1 + c_2 + c_3)\}\}$	
16 <i>Fmm2</i>	4 m_y	8 $\{\{1, 0, 0\}, \{2(1 + c_3 + c_1(2 + c_2 + c_3)), 3 + 2c_3 + 2c_1(2 + c_2 + c_3), 0\},$ $\{2(1 + c_2), 1 + 2c_2, 2(2 + c_2 + c_3)\}\}$	
16 <i>Fmm2</i>	4 m_y	9 $\{\{1, 0, 0\}, \{4 + c_2 + 3c_3 + 2c_1(2 + c_2 + c_3),$ $5 + c_2 + 3c_3 + 2c_1(2 + c_2 + c_3), 0\}, \{2(1 + c_2), 1 + 2c_2, 2(2 + c_2 + c_3)\}\}$	
16 <i>Fmm2</i>	4 m_y	10 $\{\{1, 0, 0\}, \{1 + 2c_3 + c_1(3 + 2c_2 + 2c_3), 2(1 + c_3) + c_1(3 + 2c_2 + 2c_3), 0\},$ $\{2(1 + c_2), 1 + 2c_2, 3 + 2c_2 + 2c_3\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
16 <i>Fmm2</i>	4 m_y	11 $\{\{1,0,0\}, \{2(1+c_3) + c_1(3+2c_2+2c_3), 3+2c_3 + c_1(3+2c_2+2c_3), 0\}, \{1+2c_2, 2c_2, 3+2c_2+2c_3\}\}$	
16 <i>Fmm2</i>	5 $mm2_z$	1 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{1,0,2\}\}$	
16 <i>Fmm2</i>	5 $mm2_z$	2 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,1,2\}\}$	
16 <i>Fmm2</i>	5 $mm2_z$	3 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,0,1\}\}$	
17 <i>Imm2</i>	2 2_z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
17 <i>Imm2</i>	2 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
17 <i>Imm2</i>	2 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
17 <i>Imm2</i>	2 2_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
17 <i>Imm2</i>	2 2_z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
17 <i>Imm2</i>	3 m_x	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
17 <i>Imm2</i>	3 m_x	2 $\{\{2+c_1, 0, 0\}, \{0,1,0\}, \{0,1,2+c_1\}\}$	
17 <i>Imm2</i>	3 m_x	3 $\{\{2+c_1, 0, 0\}, \{0,1,0\}, \{(2+c_1)(1+c_2), 1, (2+c_1)(2+c_2)\}\}$	
17 <i>Imm2</i>	3 m_x	4 $\{\{1+c_1, 0, 0\}, \{0,1,0\}, \{(1+c_1)(1+d_1), 1, (1+c_1)(3+d_1+d_2)\}\}$	38
17 <i>Imm2</i>	3 m_x	5 $\{\{1+c_1, 0, 0\}, \{0,1,0\}, \{1+c_1, 1, 2(1+c_1)\}\}$	
17 <i>Imm2</i>	3 m_x	6 $\{\{1+c_1, 0, 0\}, \{0,1,0\}, \{1+c_1, 1, (1+c_1)(3+c_2)\}\}$	
17 <i>Imm2</i>	3 m_x	7 $\{\{1+c_1, 0, 0\}, \{0,1,0\}, \{(1+c_1)(2+d_1), 1, (1+c_1)(3+d_1+d_2)\}\}$	42
17 <i>Imm2</i>	4 m_y	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
17 <i>Imm2</i>	4 m_y	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,3\}\}$	
17 <i>Imm2</i>	4 m_y	3 $\{\{1,0,0\}, \{0,2,0\}, \{1,2,8\}\}$	
17 <i>Imm2</i>	4 m_y	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,4+c_1\}\}$	
17 <i>Imm2</i>	4 m_y	5 $\{\{1,0,0\}, \{0,2+c_1, 0\}, \{1,0,2+c_1\}\}$	
17 <i>Imm2</i>	4 m_y	6 $\{\{1,0,0\}, \{0,2+c_1, 0\}, \{1,2+c_1, 3(2+c_1)\}\}$	
17 <i>Imm2</i>	4 m_y	7 $\{\{1,0,0\}, \{0,3+c_1, 0\}, \{1,3+c_1, 4(3+c_1)\}\}$	
17 <i>Imm2</i>	4 m_y	8 $\{\{1,0,0\}, \{0,2+c_1, 0\}, \{1, (2+c_1)(1+c_2), (2+c_1)(2+c_2)\}\}$	
17 <i>Imm2</i>	4 m_y	9 $\{\{1,0,0\}, \{0,1,0\}, \{1,2+d_1, 5+d_1+d_2\}\}$	17
17 <i>Imm2</i>	4 m_y	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,2(1+d_1), 2(5+d_1+d_2)\}\}$	16
17 <i>Imm2</i>	4 m_y	11 $\{\{1,0,0\}, \{0,2,0\}, \{1,2(2+d_1), 2(5+d_1+d_2)\}\}$	17

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
17 <i>Imm2</i>	4 m_y	12 $\{\{1,0,0\}, \{0,3+c_1,0\}, \{1,(3+c_1)(1+d_1),(3+c_1)(5+d_1+d_2)\}\}$	49
17 <i>Imm2</i>	4 m_y	13 $\{\{1,0,0\}, \{0,3+c_1,0\}, \{1,(3+c_1)(2+d_1),(3+c_1)(5+d_1+d_2)\}\}$	50
17 <i>Imm2</i>	4 m_y	14 $\{\{1,0,0\}, \{0,1,0\}, \{1,2+c_1,3+c_1\}\}$	
17 <i>Imm2</i>	4 m_y	15 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{1,1+c_1,2(1+c_1)\}\}$	
17 <i>Imm2</i>	4 m_y	16 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{1,1+c_1,(1+c_1)(3+c_2)\}\}$	
17 <i>Imm2</i>	4 m_y	17 $\{\{1,0,0\}, \{0,2+c_1,0\}, \{1,(2+c_1)(2+c_2),(2+c_1)(3+c_2)\}\}$	
17 <i>Imm2</i>	4 m_y	18 $\{\{1,0,0\}, \{0,1,0\}, \{1,3+d_1,5+d_1+d_2\}\}$	18
17 <i>Imm2</i>	4 m_y	19 $\{\{1,0,0\}, \{0,2+c_1,0\}, \{1,(2+c_1)(2+d_1),(2+c_1)(5+d_1+d_2)\}\}$	51
17 <i>Imm2</i>	4 m_y	20 $\{\{1,0,0\}, \{0,2+c_1,0\}, \{1,(2+c_1)(3+d_1),(2+c_1)(5+d_1+d_2)\}\}$	52
17 <i>Imm2</i>	5 $mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
17 <i>Imm2</i>	5 $mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 <i>Pmmm</i>	2 $\bar{1}$	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 <i>Pmmm</i>	3 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,1+c_1,2+2c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 P_{mmmm}	$3\ 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1,0,2+2c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,1+c_1,2+2c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1,0,2+2c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	7 $\{\{1,0,0\}, \{0,2,0\}, \{1+c_1,0,2+2c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	9 $\{\{2,0,0\}, \{0,1,0\}, \{0,1+c_1,2+2c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	10 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
18 P_{mmmm}	$3\ 2_z$	11 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
18 P_{mmmm}	$4\ 2_y$	1 $\{\{1,0,0\}, \{1+c_1,2+2c_1,0\}, \{0,0,1\}\}$	
18 P_{mmmm}	$4\ 2_y$	2 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
18 P_{mmmm}	$4\ 2_y$	3 $\{\{1,0,0\}, \{1+c_1,2+2c_1,0\}, \{1,0,2\}\}$	
18 P_{mmmm}	$4\ 2_y$	4 $\{\{1,0,0\}, \{1+c_1,2+2c_1,0\}, \{0,0,2\}\}$	
18 P_{mmmm}	$4\ 2_y$	5 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{1,0,2\}\}$	
18 P_{mmmm}	$4\ 2_y$	6 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{1,1,2\}\}$	
18 P_{mmmm}	$4\ 2_y$	7 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
18 P_{mmmm}	$4\ 2_y$	8 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{0,1,2\}\}$	
18 P_{mmmm}	$4\ 2_y$	9 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
18 P_{mmmm}	$4\ 2_y$	10 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
18 P_{mmmm}	$4\ 2_y$	11 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,1,2\}\}$	
18 P_{mmmm}	$5\ m_x$	1 $\{\{1,0,0\}, \{1+c_1,2(1+c_1),0\}, \{1+c_2,0,2(1+c_2)\}\}$	
18 P_{mmmm}	$5\ m_x$	2 $\{\{1,0,0\}, \{1+c_1,2(1+c_1),0\}, \{0,0,1+c_2\}\}$	
18 P_{mmmm}	$5\ m_x$	3 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{0,0,1+c_2\}\}$	
18 P_{mmmm}	$5\ m_x$	4 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{0,1+c_2,2(1+c_2)\}\}$	
18 P_{mmmm}	$5\ m_x$	5 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,0,1+c_2\}\}$	
18 P_{mmmm}	$5\ m_x$	6 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,1+c_2,2(1+c_2)\}\}$	
18 P_{mmmm}	$5\ m_x$	7 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{1+c_2,0,2(1+c_2)\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 P_{mmmm}	$5 m_x$	8 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{2(1 + c_2), 2(1 + c_2), 4(1 + c_2)\}\}$	
18 P_{mmmm}	$5 m_x$	9 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{3 + 2c_2, 3 + 2c_2, 6 + 4c_2\}\}$	
18 P_{mmmm}	$5 m_x$	10 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1 + 2c_2, 1 + 2c_2, 2 + 4c_2\}\}$	
18 P_{mmmm}	$5 m_x$	11 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{2(1 + c_2), 2(1 + c_2), 4(1 + c_2)\}\}$	
18 P_{mmmm}	$6 2_x$	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$6 2_x$	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 P_{mmmm}	$6 2_x$	3 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
18 P_{mmmm}	$6 2_x$	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$6 2_x$	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$6 2_x$	6 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$6 2_x$	7 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$6 2_x$	8 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$6 2_x$	9 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$6 2_x$	10 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$6 2_x$	11 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$7 m_y$	1 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 1 + c_2, 2(1 + c_2)\}\}$	
18 P_{mmmm}	$7 m_y$	2 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{2(1 + c_2), 2(1 + c_2), 4(1 + c_2)\}\}$	
18 P_{mmmm}	$7 m_y$	3 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + 2c_2, 1 + 2c_2, 2 + 4c_2\}\}$	
18 P_{mmmm}	$7 m_y$	4 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2(1 + c_2)\}\}$	
18 P_{mmmm}	$7 m_y$	5 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{2(1 + c_2), 0, 4(1 + c_2)\}\}$	
18 P_{mmmm}	$7 m_y$	6 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + 2c_2\}\}$	
18 P_{mmmm}	$7 m_y$	7 $\{\{1 + c_1, 0, 0\}, \{0, 1, 0\}, \{1 + 2c_2, 0, 2 + 4c_2\}\}$	
18 P_{mmmm}	$7 m_y$	8 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_2\}\}$	
18 P_{mmmm}	$7 m_y$	9 $\{\{1 + c_1, 0, 0\}, \{0, 2, 0\}, \{1 + c_2, 0, 2(1 + c_2)\}\}$	
18 P_{mmmm}	$7 m_y$	10 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_2\}\}$	
18 P_{mmmm}	$7 m_y$	11 $\{\{1 + c_1, 0, 0\}, \{1, 2, 0\}, \{1 + c_2, 0, 2(1 + c_2)\}\}$	
18 P_{mmmm}	$8 m_z$	1 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_2, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$8 m_z$	2 $\{\{1 + c_1, 0, 0\}, \{1 + c_2, 2(1 + c_2), 0\}, \{0, 0, 1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 P_{mmmm}	$8 m_z$	3 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_2, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$8 m_z$	4 $\{\{1 + c_1, 0, 0\}, \{1 + c_2, 2(1 + c_2), 0\}, \{0, 0, 2\}\}$	
18 P_{mummm}	$8 m_z$	5 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_2, 0\}, \{0, 1, 2\}\}$	
18 P_{mmmm}	$8 m_z$	6 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_2, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$8 m_z$	7 $\{\{1 + c_1, 0, 0\}, \{1 + c_2, 2(1 + c_2), 0\}, \{1, 0, 2\}\}$	
18 P_{mummm}	$8 m_z$	8 $\{\{1 + c_1, 0, 0\}, \{0, 1 + c_2, 0\}, \{1, 1, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$9 2/m_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$9 2/m_z$	7 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$9 2/m_z$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	9 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
18 P_{mummm}	$9 2/m_z$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$9 2/m_z$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$9 2/m_z$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$9 2/m_z$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$10 2/m_y$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	$10 2/m_y$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
18 P_{mmmm}	$10 2/m_y$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	$10 2/m_y$	4 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 P_{mmmm}	$10 2/m_y$	5 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	$10 2/m_y$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 P_{mmm}	10 $2/m_y$	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 P_{mmm}	10 $2/m_y$	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
18 P_{mnm}	10 $2/m_y$	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
18 P_{mmm}	10 $2/m_y$	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
18 P_{mmm}	10 $2/m_y$	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 P_{mmm}	10 $2/m_y$	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 P_{mmm}	10 $2/m_y$	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 P_{mmm}	10 $2/m_y$	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 P_{mmm}	10 $2/m_y$	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 P_{mmm}	10 $2/m_y$	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 P_{mmm}	11 $2/m_x$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 P_{mmm}	11 $2/m_x$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
18 P_{mmm}	11 $2/m_x$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
18 P_{mmm}	11 $2/m_x$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 P_{mmm}	11 $2/m_x$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 P_{mnm}	11 $2/m_x$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
18 P_{mmm}	11 $2/m_x$	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 P_{mmm}	11 $2/m_x$	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
18 P_{mmm}	11 $2/m_x$	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
18 P_{mmm}	11 $2/m_x$	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
18 P_{mmm}	11 $2/m_x$	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 P_{mmm}	11 $2/m_x$	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 P_{mmm}	11 $2/m_x$	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 P_{mmm}	11 $2/m_x$	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 P_{mmm}	11 $2/m_x$	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 P_{mmm}	11 $2/m_x$	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 P_{mmm}	12 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 P_{mmm}	12 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 $Pmmm$	12 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
18 $Pmmm$	12 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 $Pmmm$	12 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 $Pmmm$	12 222	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
18 $Pmmm$	12 222	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 $Pmmm$	12 222	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
18 $Pmmm$	12 222	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
18 $Pmmm$	12 222	10 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
18 $Pmmm$	12 222	11 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 $Pmmm$	12 222	12 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 $Pmmm$	12 222	13 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 $Pmmm$	12 222	14 $\{\{2,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 $Pmmm$	12 222	15 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 $Pmmm$	12 222	16 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 $Pmmm$	13 $mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0, 1+c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	7 $\{\{1,0,0\}, \{0,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	8 $\{\{1,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	9 $\{\{2,0,0\}, \{0,1,0\}, \{0, 1+c_1, 2+2c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	10 $\{\{2,0,0\}, \{0,1,0\}, \{0,0, 1+c_1\}\}$	
18 $Pmmm$	13 $mm2_z$	11 $\{\{2,0,0\}, \{0,2,0\}, \{0,0, 1+c_1\}\}$	
18 $Pmmm$	14 $mm2_y$	1 $\{\{1,0,0\}, \{1+c_1, 2+2c_1, 0\}, \{0,0, 1\}\}$	
18 $Pmmm$	14 $mm2_y$	2 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{0,0, 1\}\}$	
18 $Pmmm$	14 $mm2_y$	3 $\{\{1,0,0\}, \{1+c_1, 2+2c_1, 0\}, \{1,0, 2\}\}$	

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 $Pmmm$	14 $mm2_y$	4 $\{\{1,0,0\}, \{1+c_1, 2+2c_1, 0\}, \{0,0,2\}\}$	
18 $Pmmm$	14 $mm2_y$	5 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{1,0,2\}\}$	
18 $Pmnm$	14 $mm2_y$	6 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{1,1,2\}\}$	
18 $Pmmm$	14 $mm2_y$	7 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
18 $Pmmm$	14 $mm2_y$	8 $\{\{1,0,0\}, \{0,1+c_1,0\}, \{0,1,2\}\}$	
18 $Pmmm$	14 $mm2_y$	9 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
18 $Pmmm$	14 $mm2_y$	10 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
18 $Pmmm$	14 $mm2_y$	11 $\{\{2,0,0\}, \{0,1+c_1,0\}, \{0,1,2\}\}$	
18 $Pmmm$	15 $mm2_x$	1 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 $Pmmm$	15 $mm2_x$	2 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 $Pmmm$	15 $mm2_x$	3 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
18 $Pmmm$	15 $mm2_x$	4 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 $Pmmm$	15 $mm2_x$	5 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
18 $Pmmm$	15 $mm2_x$	6 $\{\{1+c_1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 $Pmmm$	15 $mm2_x$	7 $\{\{1+c_1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
18 $Pmnm$	15 $mm2_x$	8 $\{\{1+c_1,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
18 $Pmmm$	15 $mm2_x$	9 $\{\{1+c_1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
18 $Pmmm$	15 $mm2_x$	10 $\{\{1+c_1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
18 $Pmmm$	15 $mm2_x$	11 $\{\{1+c_1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
18 $Pmmm$	16 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
18 $Pmmm$	16 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
18 $Pmmm$	16 mmm	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
18 $Pmmm$	16 mmm	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
18 $Pmmm$	16 mmm	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
18 $Pmmm$	16 mmm	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
18 $Pmmm$	16 mmm	7 $\{\{1,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
18 $Pmmm$	16 mmm	8 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
18 $Pmmm$	16 mmm	9 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
18 P_{mmmm}	16 $mmmm$	10 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
18 P_{mmmm}	16 $mmmm$	11 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	16 $mmmm$	12 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	16 $mmmm$	13 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
18 P_{mmmm}	16 $mmmm$	14 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
18 P_{mmmm}	16 $mmmm$	15 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
18 P_{mmmm}	16 $mmmm$	16 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
19 C_{mmmm}	2 $\bar{1}$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 C_{mmmm}	2 $\bar{1}$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
19 C_{mmmm}	2 $\bar{1}$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 2\}\}$	
19 C_{mmmm}	2 $\bar{1}$	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1\}\}$	
19 C_{mmmm}	2 $\bar{1}$	5 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1, 0, 2\}\}$	
19 C_{mmmm}	2 $\bar{1}$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
19 C_{mmmm}	2 $\bar{1}$	7 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1\}\}$	
19 C_{mmmm}	2 $\bar{1}$	8 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 2\}\}$	
19 C_{mmmm}	3 2_z	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
19 C_{mmmm}	3 2_z	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1 + c_1\}\}$	
19 C_{mmmm}	3 2_z	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
19 C_{mmmm}	3 2_z	4 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
19 C_{mmmm}	3 2_z	5 $\{\{2, 0, 0\}, \{0, 2, 0\}, \{0, 0, 1 + c_1\}\}$	
19 C_{mmmm}	4 2_y	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1\}\}$	
19 C_{mmmm}	4 2_y	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 2\}\}$	
19 C_{mmmm}	4 2_y	3 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1, 1, 2\}\}$	
19 C_{mmmm}	5 m_x	1 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{0, 0, 1 + c_2\}\}$	
19 C_{mmmm}	5 m_x	2 $\{\{1, 0, 0\}, \{c_1, 1 + c_1, 0\}, \{1 + c_2, 1 + c_2, 2(1 + c_2)\}\}$	
19 C_{mmmm}	6 2_x	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
19 C_{mmmm}	6 2_x	2 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 1\}\}$	
19 C_{mmmm}	6 2_x	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
19 Cmmm	$6 2_x$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
19 Cmmm	$6 2_x$	5 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,0,2\}\}$	
19 Cmmm	$6 2_x$	6 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,1,2\}\}$	
19 Cmmm	$7 m_y$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
19 Cmmm	$7 m_y$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2(1+c_1)\}\}$	
19 Cmmm	$7 m_y$	3 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,0,1+c_2\}\}$	
19 Cmmm	$7 m_y$	4 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,1+c_2, 2(1+c_2)\}\}$	
19 Cmmm	$8 m_z$	1 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
19 Cmmm	$8 m_z$	2 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,1\}\}$	33
19 Cmmm	$8 m_z$	3 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
19 Cmmm	$8 m_z$	4 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,2\}\}$	33
19 Cmmm	$8 m_z$	5 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+2c_2), 2(1+c_1)(1+c_2), 0\}, \{0,1,2\}\}$	
19 Cmmm	$8 m_z$	6 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+2d_1), (1+c_1)(3+2d_1+d_2), 0\}, \{0,1,2\}\}$	54
19 Cmmm	$8 m_z$	7 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+2c_2), 2(1+c_1)(1+c_2), 0\}, \{1,0,2\}\}$	
19 Cmmm	$8 m_z$	8 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+2d_1), 2(1+c_1)(2+d_1+d_2), 0\}, \{1,0,2\}\}$	32
19 Cmmm	$8 m_z$	9 $\{\{1+c_1,0,0\}, \{(1+c_1)d_1, (1+c_1)(1+d_1+2d_2), 0\}, \{1,1,2\}\}$	66
19 Cmmm	$9 2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
19 Cmmm	$9 2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
19 Cmmm	$9 2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
19 Cmmm	$9 2/m_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
19 Cmmm	$9 2/m_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
19 Cmmm	$9 2/m_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
19 Cmmm	$9 2/m_z$	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
19 Cmmm	$9 2/m_z$	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
19 Cmmm	$10 2/m_y$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
19 Cmmm	$10 2/m_y$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
19 Cmmm	$10 2/m_y$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
19 Cmmm	$10 2/m_y$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
19 Cmmm	10 2/ m_y	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
19 Cmmm	11 2/ m_x	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
19 Cmmm	11 2/ m_x	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
19 Cmmm	11 2/ m_x	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
19 Cmmm	11 2/ m_x	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
19 Cmmm	11 2/ m_x	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
19 Cmmm	12 222	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
19 Cmmm	12 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
19 Cmmm	12 222	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
19 Cmmm	12 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
19 Cmmm	12 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
19 Cmmm	13 mm2 _z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
19 Cmmm	13 mm2 _z	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
19 Cmmm	13 mm2 _z	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
19 Cmmm	14 mm2 _y	1 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,0,1\}\}$	
19 Cmmm	14 mm2 _y	2 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,0,2\}\}$	
19 Cmmm	14 mm2 _y	3 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{1,1,2\}\}$	
19 Cmmm	15 mm2 _x	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
19 Cmmm	15 mm2 _x	2 $\{\{1,0,0\}, \{1,2+c_1, 0\}, \{0,0,1\}\}$	
19 Cmmm	15 mm2 _x	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
19 Cmmm	15 mm2 _x	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
19 Cmmm	15 mm2 _x	5 $\{\{1,0,0\}, \{1,2+c_1, 0\}, \{0,0,2\}\}$	
19 Cmmm	15 mm2 _x	6 $\{\{1,0,0\}, \{1,2+c_1, 0\}, \{0,1,2\}\}$	
19 Cmmm	16 mmm	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
19 Cmmm	16 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
19 Cmmm	16 mmm	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
19 Cmmm	16 mmm	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
19 Cmmm	16 mmm	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
20 $Fmmm$	$2 \bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$2 \bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$2 \bar{1}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
20 $Fmmm$	$2 \bar{1}$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$2 \bar{1}$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$2 \bar{1}$	6 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
20 $Fmmm$	$3 2_z$	1 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{1,0,2\}\}$	
20 $Fmmm$	$3 2_z$	2 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,1,2\}\}$	
20 $Fmmm$	$3 2_z$	3 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,0,1\}\}$	
20 $Fmmm$	$4 2_y$	1 $\{\{1,0,0\}, \{1,2,0\}, \{c_1, 0, 1+c_1\}\}$	
20 $Fmmm$	$4 2_y$	2 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, 1+c_1, 2+2c_1\}\}$	
20 $Fmmm$	$4 2_y$	3 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, 0, 1+c_1\}\}$	
20 $Fmmm$	$5 m_x$	1 $\{\{1,0,0\}, \{c_2, 1+c_2, 0\}, \{c_1, 0, 1+c_1\}\}$	
20 $Fmmm$	$5 m_x$	2 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{c_2, 1+c_2, 2(1+c_2)\}\}$	
20 $Fmmm$	$6 2_x$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$6 2_x$	2 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, c_1, 2+c_1\}\}$	
20 $Fmmm$	$6 2_x$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, c_1, 1+c_1\}\}$	
20 $Fmmm$	$6 2_x$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, c_1, 2+2c_1\}\}$	
20 $Fmmm$	$7 m_y$	1 $\{\{1,0,0\}, \{(1+c_1)c_2, 1+c_2+c_1c_2, 0\}, \{0, c_1, 1+c_1\}\}$	
20 $Fmmm$	$7 m_y$	2 $\{\{1,0,0\}, \{(1+c_1)(1+2c_2), 2+c_1+2c_2+2c_1c_2, 0\},$ $\{0, 1+2c_1, 2(1+c_1)\}\}$	
20 $Fmmm$	$7 m_y$	3 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{1,0, 2(1+c_1)\}\}$	
20 $Fmmm$	$7 m_y$	4 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{2(1+c_2), 1+2c_2, 2(2+c_1+2c_2)\}\}$	
20 $Fmmm$	$7 m_y$	5 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{3+2c_2, 2(1+c_2), 2(3+c_1+2c_2)\}\}$	
20 $Fmmm$	$7 m_y$	6 $\{\{1,0,0\}, \{1+2c_3+2c_1(1+c_2+c_3), 2(1+c_3+c_1(1+c_2+c_3)), 0\},$ $\{1+2c_2, 2c_2, 2(1+c_2+c_3)\}\}$	
20 $Fmmm$	$7 m_y$	7 $\{\{1,0,0\}, \{2+c_2+3c_3+2c_1(1+c_2+c_3),$ $3+c_2+3c_3+2c_1(1+c_2+c_3), 0\}, \{1+2c_2, 2c_2, 2(1+c_2+c_3)\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
20 $Fmmm$	$7 m_y$	8 $\{\{1,0,0\}, \{2(1+c_3+c_1(2+c_2+c_3)), 3+2c_3+2c_1(2+c_2+c_3), 0\}, \{2(1+c_2), 1+2c_2, 2(2+c_2+c_3)\}\}$	
20 $Fmmm$	$7 m_y$	9 $\{\{1,0,0\}, \{4+c_2+3c_3+2c_1(2+c_2+c_3), 5+c_2+3c_3+2c_1(2+c_2+c_3), 0\}, \{2(1+c_2), 1+2c_2, 2(2+c_2+c_3)\}\}$	
20 $Fmmm$	$7 m_y$	10 $\{\{1,0,0\}, \{1+2c_3+c_1(3+2c_2+2c_3), 2(1+c_3)+c_1(3+2c_2+2c_3), 0\}, \{2(1+c_2), 1+2c_2, 3+2c_2+2c_3\}\}$	
20 $Fmmm$	$7 m_y$	11 $\{\{1,0,0\}, \{2(1+c_3)+c_1(3+2c_2+2c_3), 3+2c_3+c_1(3+2c_2+2c_3), 0\}, \{1+2c_2, 2c_2, 3+2c_2+2c_3\}\}$	
20 $Fmmm$	$8 m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{d_1, d_2, 1+d_1+d_2\}\}$	3
20 $Fmmm$	$8 m_z$	2 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, c_1, 2+c_1\}\}$	
20 $Fmmm$	$8 m_z$	3 $\{\{1,0,0\}, \{1,2(1+c_1), 0\}, \{c_1, 0, 1+c_1\}\}$	
20 $Fmmm$	$8 m_z$	4 $\{\{1,0,0\}, \{1,2(3+d_1+d_2), 0\}, \{5+2d_1+3d_2, 3+d_1+d_2, 6+2d_1+3d_2\}\}$	25*
20 $Fmmm$	$8 m_z$	5 $\{\{1,0,0\}, \{1,2(2+c_1), 0\}, \{5+3c_1+2(2+c_1)d_1+2(2+c_1)d_2, 2(2+c_1)d_1, (2+c_1)(3+2d_1+2d_2)\}\}$	58
20 $Fmmm$	$8 m_z$	6 $\{\{1,0,0\}, \{1,2(2+c_1), 0\}, \{5+4d_1+2d_2+c_1(3+2d_1+d_2), (2+c_1)(1+2d_1), (2+c_1)(3+2d_1+d_2)\}\}$	55
20 $Fmmm$	$8 m_z$	7 $\{\{1,0,0\}, \{1,3+c_1, 0\}, \{2+c_1+(3+c_1)d_1+(3+c_1)d_2, (3+c_1)d_1, (3+c_1)(1+d_1+d_2)\}\}$	30
20 $Fmmm$	$8 m_z$	8 $\{\{1,0,0\}, \{1,2(1+d_1), 0\}, \{3+3d_1+2(1+d_1)d_2+d_3, (1+d_1)(1+2d_2), 4+3d_1+2(1+d_1)d_2+d_3\}\}$	68
20 $Fmmm$	$8 m_z$	9 $\{\{1,0,0\}, \{1,2+d_1, 0\}, \{2+d_1+(2+d_1)d_2+d_3, (2+d_1)d_2, 3+d_1+(2+d_1)d_2+d_3\}\}$	67
20 $Fmmm$	$8 m_z$	10 $\{\{1,0,0\}, \{1,2(2+d_1+d_2), 0\}, \{4+2d_1+3d_2+2(2+d_1+d_2)d_3, (2+d_1+d_2)(1+2d_3), 5+2d_1+3d_2+2(2+d_1+d_2)d_3\}\}$	72*
20 $Fmmm$	$8 m_z$	11 $\{\{1,0,0\}, \{1,2(3+d_1+d_2), 0\}, \{6+2d_1+3d_2+2(3+d_1+d_2)d_3, (3+d_1+d_2)(1+2d_3), 7+2d_1+3d_2+2(3+d_1+d_2)d_3\}\}$	73*
20 $Fmmm$	$8 m_z$	12 $\{\{1,0,0\}, \{1,2(3+d_1+d_2), 0\}, \{5+2d_1+3d_2+2(3+d_1+d_2)(1+d_3), (3+d_1+d_2)(3+2d_3), 6+2d_1+3d_2+2(3+d_1+d_2)(1+d_3)\}\}$	74*

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
20 $Fmmm$	$8 m_z$	13 $\{\{1,0,0\}, \{1,4+2d_1+d_2,0\}, \{2+d_1+d_2+(4+2d_1+d_2)(1+d_3), (4+2d_1+d_2)(1+d_3), 3+d_1+d_2+(4+2d_1+d_2)(1+d_3)\}\}$	69*
20 $Fmmm$	$8 m_z$	14 $\{\{1,0,0\}, \{1,5+2d_1+d_2,0\}, \{2+d_1+d_2+(5+2d_1+d_2)(1+d_3), (5+2d_1+d_2)(1+d_3), 3+d_1+d_2+(5+2d_1+d_2)(1+d_3)\}\}$	70*
20 $Fmmm$	$8 m_z$	15 $\{\{1,0,0\}, \{1,6+2d_1+d_2,0\}, \{2+d_1+d_2+(6+2d_1+d_2)(1+d_3), (6+2d_1+d_2)(1+d_3), 3+d_1+d_2+(6+2d_1+d_2)(1+d_3)\}\}$	71*
20 $Fmmm$	$9 2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
20 $Fmmm$	$9 2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$9 2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$9 2/m_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$9 2/m_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$10 2/m_y$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
20 $Fmmm$	$10 2/m_y$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$10 2/m_y$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$10 2/m_y$	4 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$10 2/m_y$	5 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$11 2/m_x$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
20 $Fmmm$	$11 2/m_x$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$11 2/m_x$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$11 2/m_x$	4 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
20 $Fmmm$	$11 2/m_x$	5 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
20 $Fmmm$	12 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
20 $Fmmm$	12 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
20 $Fmmm$	12 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
20 $Fmmm$	12 222	4 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
20 $Fmmm$	12 222	5 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
20 $Fmmm$	$13 mm2_z$	1 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{1,0,2\}\}$	
20 $Fmmm$	$13 mm2_z$	2 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,1,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
20 $Fmmm$	13 $mm2_z$	3 $\{\{1,0,0\}, \{c_1, 1+c_1, 0\}, \{0,0,1\}\}$	
20 $Fmmm$	14 $mm2_y$	1 $\{\{1,0,0\}, \{1,2,0\}, \{c_1, 0, 1+c_1\}\}$	
20 $Fmmm$	14 $mm2_y$	2 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, 1+c_1, 2+2c_1\}\}$	
20 $Fmmm$	14 $mm2_y$	3 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, 0, 1+c_1\}\}$	
20 $Fmmm$	15 $mm2_x$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
20 $Fmmm$	15 $mm2_x$	2 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, c_1, 2+c_1\}\}$	
20 $Fmmm$	15 $mm2_x$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0, c_1, 1+c_1\}\}$	
20 $Fmmm$	15 $mm2_x$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, c_1, 2+2c_1\}\}$	
20 $Fmmm$	16 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
20 $Fmmm$	16 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,0,2\}\}$	
20 $Fmmm$	16 mmm	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
20 $Fmmm$	16 mmm	4 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
20 $Fmmm$	16 mmm	5 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
21 $Immm$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 $Immm$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
21 $Iumm$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
21 $Iumm$	2 $\bar{1}$	4 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
21 $Iumm$	2 $\bar{1}$	5 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
21 $Iumm$	2 $\bar{1}$	6 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
21 $Iumm$	3 2_z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
21 $Iumm$	3 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 $Iumm$	3 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
21 $Iumm$	3 2_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
21 $Iumm$	3 2_z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
21 $Iumm$	4 2_y	1 $\{\{1,0,0\}, \{0,2,0\}, \{1,0,2\}\}$	
21 $Iumm$	4 2_y	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 $Iumm$	4 2_y	3 $\{\{1,0,0\}, \{0,2,0\}, \{3+2c_1, 2, 2(2+c_1)\}\}$	
21 $Iumm$	4 2_y	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+4c_1, 3+2c_1, 4(1+c_1)\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
21 <i>Immm</i>	4 2_y	5 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1, 2+c_1\}\}$	
21 <i>Immm</i>	5 m_x	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	5 m_x	2 $\{\{2+c_1,0,0\}, \{0,1,0\}, \{0,1,2+c_1\}\}$	
21 <i>Immm</i>	5 m_x	3 $\{\{2+c_1,0,0\}, \{0,1,0\}, \{(2+c_1)(1+c_2), 1, (2+c_1)(2+c_2)\}\}$	
21 <i>Immm</i>	5 m_x	4 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{(1+c_1)(1+d_1), 1, (1+c_1)(3+d_1+d_2)\}\}$	38
21 <i>Immm</i>	5 m_x	5 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{1+c_1, 1, 2(1+c_1)\}\}$	
21 <i>Immm</i>	5 m_x	6 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{1+c_1, 1, (1+c_1)(3+c_2)\}\}$	
21 <i>Immm</i>	5 m_x	7 $\{\{1+c_1,0,0\}, \{0,1,0\}, \{(1+c_1)(2+d_1), 1, (1+c_1)(3+d_1+d_2)\}\}$	42
21 <i>Immm</i>	6 2_x	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	6 2_x	2 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+4c_1, 4(1+c_1)\}\}$	
21 <i>Immm</i>	6 2_x	3 $\{\{1,0,0\}, \{0,1,0\}, \{1, 1+c_1, 2+c_1\}\}$	
21 <i>Immm</i>	6 2_x	4 $\{\{2,0,0\}, \{0,1,0\}, \{0,1,2\}\}$	
21 <i>Immm</i>	6 2_x	5 $\{\{2,0,0\}, \{0,1,0\}, \{2, 3+2c_1, 2(2+c_1)\}\}$	
21 <i>Immm</i>	7 m_y	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	7 m_y	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,3\}\}$	
21 <i>Immm</i>	7 m_y	3 $\{\{1,0,0\}, \{0,2,0\}, \{1,2,8\}\}$	
21 <i>Immm</i>	7 m_y	4 $\{\{1,0,0\}, \{0,1,0\}, \{1, 1, 4+c_1\}\}$	
21 <i>Immm</i>	7 m_y	5 $\{\{1,0,0\}, \{0, 2+c_1, 0\}, \{1, 0, 2+c_1\}\}$	
21 <i>Immm</i>	7 m_y	6 $\{\{1,0,0\}, \{0, 2+c_1, 0\}, \{1, 2+c_1, 3(2+c_1)\}\}$	
21 <i>Immm</i>	7 m_y	7 $\{\{1,0,0\}, \{0, 3+c_1, 0\}, \{1, 3+c_1, 4(3+c_1)\}\}$	
21 <i>Immm</i>	7 m_y	8 $\{\{1,0,0\}, \{0, 2+c_1, 0\}, \{1, (2+c_1)(1+c_2), (2+c_1)(2+c_2)\}\}$	
21 <i>Immm</i>	7 m_y	9 $\{\{1,0,0\}, \{0,1,0\}, \{1, 2+d_1, 5+d_1+d_2\}\}$	17
21 <i>Immm</i>	7 m_y	10 $\{\{1,0,0\}, \{0,2,0\}, \{1, 2(1+d_1), 2(5+d_1+d_2)\}\}$	16
21 <i>Immm</i>	7 m_y	11 $\{\{1,0,0\}, \{0,2,0\}, \{1, 2(2+d_1), 2(5+d_1+d_2)\}\}$	17
21 <i>Immm</i>	7 m_y	12 $\{\{1,0,0\}, \{0, 3+c_1, 0\}, \{1, (3+c_1)(1+d_1), (3+c_1)(5+d_1+d_2)\}\}$	49
21 <i>Immm</i>	7 m_y	13 $\{\{1,0,0\}, \{0, 3+c_1, 0\}, \{1, (3+c_1)(2+d_1), (3+c_1)(5+d_1+d_2)\}\}$	50
21 <i>Immm</i>	7 m_y	14 $\{\{1,0,0\}, \{0,1,0\}, \{1, 2+c_1, 3+c_1\}\}$	
21 <i>Immm</i>	7 m_y	15 $\{\{1,0,0\}, \{0, 1+c_1, 0\}, \{1, 1+c_1, 2(1+c_1)\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
21 <i>Immm</i>	$7 m_y$	16 $\{\{1, 0, 0\}, \{0, 1 + c_1, 0\}, \{1, 1 + c_1, (1 + c_1)(3 + c_2)\}\}$	
21 <i>Immm</i>	$7 m_y$	17 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(2 + c_2), (2 + c_1)(3 + c_2)\}\}$	
21 <i>Inumm</i>	$7 m_y$	18 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 3 + d_1, 5 + d_1 + d_2\}\}$	18
21 <i>Immm</i>	$7 m_y$	19 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(2 + d_1), (2 + c_1)(5 + d_1 + d_2)\}\}$	51
21 <i>Immm</i>	$7 m_y$	20 $\{\{1, 0, 0\}, \{0, 2 + c_1, 0\}, \{1, (2 + c_1)(3 + d_1), (2 + c_1)(5 + d_1 + d_2)\}\}$	52
21 <i>Immm</i>	$8 m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 <i>Immm</i>	$8 m_z$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1 + d_1, 1 + d_2, 2 + d_1 + d_2\}\}$	4
21 <i>Immm</i>	$8 m_z$	3 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
21 <i>Immm</i>	$8 m_z$	4 $\{\{1, 0, 0\}, \{1, 3, 0\}, \{0, 3, 6\}\}$	
21 <i>Immm</i>	$8 m_z$	5 $\{\{1, 0, 0\}, \{1, 2 + c_1, 0\}, \{0, 0, 2 + c_1\}\}$	
21 <i>Immm</i>	$8 m_z$	6 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 2, 2(2 + c_1)\}\}$	
21 <i>Immm</i>	$8 m_z$	7 $\{\{1, 0, 0\}, \{1, 4 + c_1, 0\}, \{0, 4 + c_1, 2(4 + c_1)\}\}$	
21 <i>Immm</i>	$8 m_z$	8 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 2(2 + d_1), 2(3 + d_1 + d_2)\}\}$	9
21 <i>Immm</i>	$8 m_z$	9 $\{\{1, 0, 0\}, \{1, 3, 0\}, \{0, 3(1 + d_1), 3(3 + d_1 + d_2)\}\}$	6
21 <i>Immm</i>	$8 m_z$	10 $\{\{1, 0, 0\}, \{1, 3, 0\}, \{0, 3(2 + d_1), 3(3 + d_1 + d_2)\}\}$	9
21 <i>Inumm</i>	$8 m_z$	11 $\{\{1, 0, 0\}, \{1, 4 + c_1, 0\}, \{0, (4 + c_1)(1 + d_1), (4 + c_1)(3 + d_1 + d_2)\}\}$	38
21 <i>Immm</i>	$8 m_z$	12 $\{\{1, 0, 0\}, \{1, 4 + c_1, 0\}, \{0, (4 + c_1)(2 + d_1), (4 + c_1)(3 + d_1 + d_2)\}\}$	42
21 <i>Immm</i>	$9 2/m_z$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 <i>Immm</i>	$9 2/m_z$	2 $\{\{1, 0, 0\}, \{1, 2, 0\}, \{0, 0, 2\}\}$	
21 <i>Immm</i>	$9 2/m_z$	3 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 <i>Immm</i>	$10 2/m_y$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 <i>Immm</i>	$10 2/m_y$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 <i>Immm</i>	$10 2/m_y$	3 $\{\{1, 0, 0\}, \{0, 2, 0\}, \{1, 0, 2\}\}$	
21 <i>Immm</i>	$11 2/m_x$	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	
21 <i>Immm</i>	$11 2/m_x$	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$	
21 <i>Immm</i>	$11 2/m_x$	3 $\{\{2, 0, 0\}, \{0, 1, 0\}, \{0, 1, 2\}\}$	
21 <i>Immm</i>	12 222	1 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{3, 3, 4\}\}$	
21 <i>Immm</i>	12 222	2 $\{\{1, 0, 0\}, \{0, 1, 0\}, \{1, 1, 2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
21 <i>Immm</i>	12 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	12 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
21 <i>Immm</i>	12 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
21 <i>Immm</i>	12 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	13 <i>mm2_z</i>	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	13 <i>mm2_z</i>	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
21 <i>Immm</i>	14 <i>mm2_y</i>	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	14 <i>mm2_y</i>	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1, 2+c_1\}\}$	
21 <i>Immm</i>	15 <i>mm2_x</i>	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
21 <i>Immm</i>	15 <i>mm2_x</i>	2 $\{\{1,0,0\}, \{0,1,0\}, \{1, 1+c_1, 2+c_1\}\}$	
21 <i>Immm</i>	16 <i>mmm</i>	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
21 <i>Immm</i>	16 <i>mmm</i>	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
22 <i>P4</i>	2 2 _z	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
22 <i>P4</i>	2 2 _z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
22 <i>P4</i>	2 2 _z	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
22 <i>P4</i>	2 2 _z	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
22 <i>P4</i>	2 2 _z	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
22 <i>P4</i>	3 4	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
22 <i>P4</i>	3 4	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
22 <i>P4</i>	3 4	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
23 <i>I4</i>	2 2 _z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
23 <i>I4</i>	2 2 _z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
23 <i>I4</i>	2 2 _z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
23 <i>I4</i>	2 2 _z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
23 <i>I4</i>	2 2 _z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
23 <i>I4</i>	3 4	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
23 <i>I4</i>	3 4	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
24 <i>P$\bar{4}$</i>	2 2 _z	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
24 $P\bar{4}$	2 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
24 $P\bar{4}$	2 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1,0,2+2c_1\}\}$	
24 $P\bar{4}$	2 2_z	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
24 $P\bar{4}$	2 2_z	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
24 $P\bar{4}$	3 $\bar{4}$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
24 $P\bar{4}$	3 $\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
24 $P\bar{4}$	3 $\bar{4}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
24 $P\bar{4}$	3 $\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
24 $P\bar{4}$	3 $\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
25 $I\bar{4}$	2 2_z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
25 $I\bar{4}$	2 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
25 $I\bar{4}$	2 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
25 $I\bar{4}$	2 2_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
25 $I\bar{4}$	2 2_z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
25 $I\bar{4}$	3 $\bar{4}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
25 $I\bar{4}$	3 $\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
25 $I\bar{4}$	3 $\bar{4}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
25 $I\bar{4}$	3 $\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
25 $I\bar{4}$	3 $\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
25 $I\bar{4}$	3 $\bar{4}$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
26 $P4/m$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
26 $P4/m$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
26 $P4/m$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
26 $P4/m$	2 $\bar{1}$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
26 $P4/m$	2 $\bar{1}$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
26 $P4/m$	2 $\bar{1}$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
26 $P4/m$	2 $\bar{1}$	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
26 $P4/m$	2 $\bar{1}$	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
26 $P4/m$	$3 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
26 $P4/m$	$3 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
26 $P4/m$	$3 2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
26 $P4/m$	$3 2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
26 $P4/m$	$3 2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
26 $P4/m$	$4 m_z$	1 $\{\{1+c_1, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 1\}\}$	
26 $P4/m$	$4 m_z$	2 $\{\{1+c_1, 0, 0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0, 0, 1\}\}$	35
26 $P4/m$	$4 m_z$	3 $\{\{1+c_1, 0, 0\}, \{0, 1+c_1, 0\}, \{0, 0, 2\}\}$	
26 $P4/m$	$4 m_z$	4 $\{\{1+c_1, 0, 0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0, 0, 2\}\}$	35
26 $P4/m$	$4 m_z$	5 $\{\{1+c_1, 0, 0\}, \{(1+c_1)(1+2d_1), (1+c_1)(2+2d_1+d_2), 0\}, \{0, 1, 2\}\}$	53
26 $P4/m$	$4 m_z$	6 $\{\{1+c_1, 0, 0\}, \{(1+c_1)(1+2d_1), 2(1+c_1)(1+d_1+d_2), 0\}, \{1, 0, 2\}\}$	31
26 $P4/m$	$4 m_z$	7 $\{\{1+c_1, 0, 0\}, \{0, 1+c_1, 0\}, \{1, 1, 2\}\}$	
26 $P4/m$	$4 m_z$	8 $\{\{1+c_1, 0, 0\}, \{(1+c_1)d_1, (1+c_1)(3+d_1+2d_2), 0\}, \{1, 1, 2\}\}$	64
26 $P4/m$	$5 2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
26 $P4/m$	$5 2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
26 $P4/m$	$5 2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
26 $P4/m$	$5 2/m_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
26 $P4/m$	$5 2/m_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
26 $P4/m$	$5 2/m_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
26 $P4/m$	$5 2/m_z$	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
26 $P4/m$	$5 2/m_z$	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
26 $P4/m$	$6 \bar{4}$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
26 $P4/m$	$6 \bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
26 $P4/m$	$6 \bar{4}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
26 $P4/m$	$6 \bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
26 $P4/m$	$6 \bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
26 $P4/m$	7 4	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
26 $P4/m$	7 4	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
26 $P4/m$	7 4	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
26 $P4/m$	8 $4/m$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
26 $P4/m$	8 $4/m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
26 $P4/m$	8 $4/m$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
26 $P4/m$	8 $4/m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
26 $P4/m$	8 $4/m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
27 $I4/m$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
27 $I4/m$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
27 $I4/m$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
27 $I4/m$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
27 $I4/m$	3 2_z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
27 $I4/m$	3 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
27 $I4/m$	3 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
27 $I4/m$	3 2_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
27 $I4/m$	3 2_z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
27 $I4/m$	4 m_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
27 $I4/m$	4 m_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+d_1, 1+d_2, 2+d_1+d_2\}\}$	5
27 $I4/m$	4 m_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
27 $I4/m$	4 m_z	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,2,4\}\}$	
27 $I4/m$	4 m_z	5 $\{\{1,0,0\}, \{1,3,0\}, \{0,3,6\}\}$	
27 $I4/m$	4 m_z	6 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,0,2+c_1\}\}$	
27 $I4/m$	4 m_z	7 $\{\{1,0,0\}, \{1,4+c_1,0\}, \{0,4+c_1,2(4+c_1)\}\}$	
27 $I4/m$	4 m_z	8 $\{\{1,0,0\}, \{1,2,0\}, \{0,2(2+d_1), 2(3+d_1+d_2)\}\}$	10
27 $I4/m$	4 m_z	9 $\{\{1,0,0\}, \{1,3,0\}, \{0,3(1+d_1), 3(3+d_1+d_2)\}\}$	7
27 $I4/m$	4 m_z	10 $\{\{1,0,0\}, \{1,3,0\}, \{0,3(2+d_1), 3(3+d_1+d_2)\}\}$	10
27 $I4/m$	4 m_z	11 $\{\{1,0,0\}, \{1,4+c_1,0\}, \{0, (4+c_1)(1+d_1), (4+c_1)(3+d_1+d_2)\}\}$	39
27 $I4/m$	4 m_z	12 $\{\{1,0,0\}, \{1,4+c_1,0\}, \{0, (4+c_1)(2+d_1), (4+c_1)(3+d_1+d_2)\}\}$	43
27 $I4/m$	5 $2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
27 $I4/m$	$5 2/m_z$	2 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
27 $I4/m$	$5 2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
27 $I4/m$	$6 \bar{4}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
27 $I4/m$	$6 \bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
27 $I4/m$	$6 \bar{4}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
27 $I4/m$	$6 \bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
27 $I4/m$	$6 \bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
27 $I4/m$	$6 \bar{4}$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
27 $I4/m$	$7 4$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
27 $I4/m$	$7 4$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2 + c_1\}\}$	
27 $I4/m$	$8 4/m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
27 $I4/m$	$8 4/m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
28 $P422$	$2 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1 + c_1, 1 + c_1, 2 + 2c_1\}\}$	
28 $P422$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1 + c_1\}\}$	
28 $P422$	$2 2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1 + c_1, 0, 2 + 2c_1\}\}$	
28 $P422$	$2 2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1 + c_1\}\}$	
28 $P422$	$2 2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1 + c_1\}\}$	
28 $P422$	$3 222$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
28 $P422$	$3 222$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
28 $P422$	$3 222$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
28 $P422$	$3 222$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
28 $P422$	$3 222$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
28 $P422$	$3 222$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
28 $P422$	$3 222$	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
28 $P422$	$3 222$	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
28 $P422$	$4 222_d$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
28 $P422$	$4 222_d$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
28 $P422$	$4 222_d$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
28 P422	4 222 _d	4 {{1,0,0},{0,1,0},{1,1,2}}	
28 P422	4 222 _d	5 {{1,0,0},{0,1,0},{0,0,2}}	
28 P422	5 4	1 {{1,0,0},{1,2,0},{0,0,1+c ₁ }}	
28 P422	5 4	2 {{1,0,0},{0,1,0},{1+c ₁ ,1+c ₁ ,2+2c ₁ }}	
28 P422	5 4	3 {{1,0,0},{0,1,0},{0,0,1+c ₁ }}	
28 P422	6 422	1 {{1,0,0},{1,2,0},{0,0,1}}	
28 P422	6 422	2 {{1,0,0},{0,1,0},{0,0,1}}	
28 P422	6 422	3 {{1,0,0},{1,2,0},{0,0,2}}	
28 P422	6 422	4 {{1,0,0},{0,1,0},{1,1,2}}	
28 P422	6 422	5 {{1,0,0},{0,1,0},{0,0,2}}	
29 I422	2 2 _z	1 {{1,0,0},{1,2,0},{0,0,2}}	
29 I422	2 2 _z	2 {{1,0,0},{0,1,0},{0,0,1}}	
29 I422	2 2 _z	3 {{1,0,0},{1,2,0},{2,2,2(2+c ₁)}}	
29 I422	2 2 _z	4 {{1,0,0},{0,1,0},{3+2c ₁ ,3+2c ₁ ,4(1+c ₁)}}	
29 I422	2 2 _z	5 {{1,0,0},{0,1,0},{1,1,2+c ₁ }}	
29 I422	3 222	1 {{1,0,0},{0,1,0},{3,3,4}}	
29 I422	3 222	2 {{1,0,0},{0,1,0},{1,1,2}}	
29 I422	3 222	3 {{1,0,0},{0,1,0},{0,0,1}}	
29 I422	3 222	4 {{1,0,0},{0,1,0},{3,3,4}}	
29 I422	3 222	5 {{1,0,0},{0,1,0},{1,1,2}}	
29 I422	3 222	6 {{1,0,0},{0,1,0},{0,0,1}}	
29 I422	4 222 _d	1 {{1,0,0},{0,1,0},{0,0,1}}	
29 I422	4 222 _d	2 {{1,0,0},{1,2,0},{0,0,2}}	
29 I422	4 222 _d	3 {{1,0,0},{0,1,0},{1,1,2}}	
29 I422	5 4	1 {{1,0,0},{0,1,0},{0,0,1}}	
29 I422	5 4	2 {{1,0,0},{0,1,0},{1,1,2+c ₁ }}	
29 I422	6 422	1 {{1,0,0},{0,1,0},{1,1,2}}	
29 I422	6 422	2 {{1,0,0},{0,1,0},{0,0,1}}	

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
30 $P4mm$	$2 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
30 $P4mm$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$2 2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
30 $P4mm$	$2 2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$2 2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$3 mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
30 $P4mm$	$3 mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$3 mm2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
30 $P4mm$	$3 mm2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$3 mm2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$4 mm2_d$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$4 mm2_d$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
30 $P4mm$	$4 mm2_d$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$5 4$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$5 4$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
30 $P4mm$	$5 4$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$6 4mm$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
30 $P4mm$	$6 4mm$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
30 $P4mm$	$6 4mm$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
31 $I4mm$	$2 2_z$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
31 $I4mm$	$2 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
31 $I4mm$	$2 2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
31 $I4mm$	$2 2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
31 $I4mm$	$2 2_z$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
31 $I4mm$	$3 mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
31 $I4mm$	$3 mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
31 $I4mm$	$4 mm2_d$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
31 $I4mm$	$4 mm2_d$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
31 $I4mm$	4 $mm2_d$	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
31 $I4mm$	4 $mm2_d$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
31 $I4mm$	4 $mm2_d$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
31 $I4mm$	5 4	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
31 $I4mm$	5 4	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
31 $I4mm$	6 $4mm$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
31 $I4mm$	6 $4mm$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
32 $P\bar{4}2m$	2 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
32 $P\bar{4}2m$	2 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
32 $P\bar{4}2m$	2 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
32 $P\bar{4}2m$	2 2_z	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
32 $P\bar{4}2m$	2 2_z	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
32 $P\bar{4}2m$	3 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
32 $P\bar{4}2m$	3 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
32 $P\bar{4}2m$	3 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
32 $P\bar{4}2m$	3 222	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
32 $P\bar{4}2m$	3 222	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
32 $P\bar{4}2m$	3 222	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
32 $P\bar{4}2m$	3 222	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
32 $P\bar{4}2m$	3 222	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
32 $P\bar{4}2m$	4 $mm2_d$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
32 $P\bar{4}2m$	4 $mm2_d$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
32 $P\bar{4}2m$	4 $mm2_d$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
32 $P\bar{4}2m$	5 $\bar{4}$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
32 $P\bar{4}2m$	5 $\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
32 $P\bar{4}2m$	5 $\bar{4}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
32 $P\bar{4}2m$	5 $\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
32 $P\bar{4}2m$	5 $\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
32 $P\bar{4}2m$	6 $\bar{4}2m$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
32 $P\bar{4}2m$	6 $\bar{4}2m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
32 $P\bar{4}2m$	6 $\bar{4}2m$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
32 $P\bar{4}2m$	6 $\bar{4}2m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
32 $P\bar{4}2m$	6 $\bar{4}2m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
33 $P\bar{4}m2$	2 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
33 $P\bar{4}m2$	2 2_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
33 $P\bar{4}m2$	2 2_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
33 $P\bar{4}m2$	2 2_z	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
33 $P\bar{4}m2$	2 2_z	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
33 $P\bar{4}m2$	3 $mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
33 $P\bar{4}m2$	3 $mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
33 $P\bar{4}m2$	3 $mm2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
33 $P\bar{4}m2$	3 $mm2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
33 $P\bar{4}m2$	3 $mm2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
33 $P\bar{4}m2$	4 222_d	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
33 $P\bar{4}m2$	4 222_d	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
33 $P\bar{4}m2$	4 222_d	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
33 $P\bar{4}m2$	4 222_d	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
33 $P\bar{4}m2$	4 222_d	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
33 $P\bar{4}m2$	5 $\bar{4}$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
33 $P\bar{4}m2$	5 $\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
33 $P\bar{4}m2$	5 $\bar{4}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
33 $P\bar{4}m2$	5 $\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
33 $P\bar{4}m2$	5 $\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
33 $P\bar{4}m2$	6 $\bar{4}m2$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
33 $P\bar{4}m2$	6 $\bar{4}m2$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
33 $P\bar{4}m2$	6 $\bar{4}m2$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
33 $P\bar{4}m2$	$6\bar{4}m2$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
33 $P\bar{4}m2$	$6\bar{4}m2$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
34 $I\bar{4}m2$	22_z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
34 $I\bar{4}m2$	22_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
34 $I\bar{4}m2$	22_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
34 $I\bar{4}m2$	22_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
34 $I\bar{4}m2$	22_z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
34 $I\bar{4}m2$	$3mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
34 $I\bar{4}m2$	$3mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
34 $I\bar{4}m2$	4222_d	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
34 $I\bar{4}m2$	4222_d	2 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
34 $I\bar{4}m2$	4222_d	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
34 $I\bar{4}m2$	$5\bar{4}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
34 $I\bar{4}m2$	$5\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
34 $I\bar{4}m2$	$5\bar{4}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
34 $I\bar{4}m2$	$5\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
34 $I\bar{4}m2$	$5\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
34 $I\bar{4}m2$	$5\bar{4}$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
34 $I\bar{4}m2$	$6\bar{4}m2$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
34 $I\bar{4}m2$	$6\bar{4}m2$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
35 $I\bar{4}2m$	22_z	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
35 $I\bar{4}2m$	22_z	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
35 $I\bar{4}2m$	22_z	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
35 $I\bar{4}2m$	22_z	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
35 $I\bar{4}2m$	22_z	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
35 $I\bar{4}2m$	3222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
35 $I\bar{4}2m$	3222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
35 $I\bar{4}2m$	3222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
35 $I\bar{4}2m$	3 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
35 $I\bar{4}2m$	3 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
35 $I\bar{4}2m$	3 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
35 $I\bar{4}2m$	4 $mm2_d$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
35 $I\bar{4}2m$	4 $mm2_d$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
35 $I\bar{4}2m$	4 $mm2_d$	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
35 $I\bar{4}2m$	4 $mm2_d$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
35 $I\bar{4}2m$	4 $mm2_d$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
35 $I\bar{4}2m$	5 $\bar{4}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
35 $I\bar{4}2m$	5 $\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
35 $I\bar{4}2m$	5 $\bar{4}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
35 $I\bar{4}2m$	5 $\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
35 $I\bar{4}2m$	5 $\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
35 $I\bar{4}2m$	5 $\bar{4}$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
35 $I\bar{4}2m$	6 $\bar{4}2m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
35 $I\bar{4}2m$	6 $\bar{4}2m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
35 $I\bar{4}2m$	6 $\bar{4}2m$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
35 $I\bar{4}2m$	6 $\bar{4}2m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
35 $I\bar{4}2m$	6 $\bar{4}2m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
35 $I\bar{4}2m$	6 $\bar{4}2m$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	2 $\bar{1}$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	2 $\bar{1}$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
36 $P4/mmm$	2 $\bar{1}$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	2 $\bar{1}$	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	2 $\bar{1}$	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
36 $P4/mmm$	$3 2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
36 $P4/mmm$	$3 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	$3 2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
36 $P4/mmm$	$3 2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	$3 2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	$4 m_z$	1 $\{\{2(1+c_1), 0, 0\}, \{0, 2(1+c_1), 0\}, \{0, 0, 1\}\}$	
36 $P4/mmm$	$4 m_z$	2 $\{\{2(1+c_1), 0, 0\}, \{2(1+c_1), 4(1+c_1), 0\}, \{0, 0, 1\}\}$	
36 $P4/mmm$	$4 m_z$	3 $\{\{1+2c_1, 0, 0\}, \{0, 1+2c_1, 0\}, \{0, 0, 1\}\}$	
36 $P4/mmm$	$4 m_z$	4 $\{\{1+2c_1, 0, 0\}, \{1+2c_1, 2+4c_1, 0\}, \{0, 0, 1\}\}$	
36 $P4/mmm$	$4 m_z$	5 $\{\{2(1+c_1), 0, 0\}, \{2(1+c_1)(2+d_1), 4(1+c_1)(2+d_1), 0\}, \{0, 0, 1\}\}$	2*
36 $P4/mmm$	$4 m_z$	6 $\{\{1+2c_1, 0, 0\}, \{(1+2c_1)(2+d_1), 2(1+2c_1)(2+d_1), 0\}, \{0, 0, 1\}\}$	2*
36 $P4/mmm$	$4 m_z$	7 $\{\{2(1+c_1), 0, 0\}, \{0, 2(1+c_1), 0\}, \{0, 0, 2\}\}$	
36 $P4/mmm$	$4 m_z$	8 $\{\{2(1+c_1), 0, 0\}, \{2(1+c_1), 4(1+c_1), 0\}, \{0, 0, 2\}\}$	
36 $P4/mmm$	$4 m_z$	9 $\{\{1+2c_1, 0, 0\}, \{0, 1+2c_1, 0\}, \{0, 0, 2\}\}$	
36 $P4/mmm$	$4 m_z$	10 $\{\{1+2c_1, 0, 0\}, \{1+2c_1, 2+4c_1, 0\}, \{0, 0, 2\}\}$	
36 $P4/mmm$	$4 m_z$	11 $\{\{2(1+c_1), 0, 0\}, \{2(1+c_1)(2+d_1), 4(1+c_1)(2+d_1), 0\}, \{0, 0, 2\}\}$	2*
36 $P4/mmm$	$4 m_z$	12 $\{\{1+2c_1, 0, 0\}, \{(1+2c_1)(2+d_1), 2(1+2c_1)(2+d_1), 0\}, \{0, 0, 2\}\}$	2*
36 $P4/mmm$	$4 m_z$	13 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
36 $P4/mmm$	$4 m_z$	14 $\{\{2+c_1, 0, 0\}, \{2+c_1, 2(2+c_1), 0\}, \{1,0,2\}\}$	
36 $P4/mmm$	$4 m_z$	15 $\{\{1,0,0\}, \{2+d_1, 2(2+d_1), 0\}, \{1,0,2\}\}$	1*
36 $P4/mmm$	$4 m_z$	16 $\{\{1+c_1, 0, 0\}, \{0, 1+c_1, 0\}, \{1,1,2\}\}$	
36 $P4/mmm$	$5 2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	$5 2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	$5 2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	$5 2/m_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	$5 2/m_z$	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
36 $P4/mmm$	$5 2/m_z$	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	$5 2/m_z$	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
36 $P4/mmm$	$5 2/m_z$	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	6 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	6 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	6 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	6 222	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	6 222	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
36 $P4/mmm$	6 222	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	6 222	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	6 222	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	$7 mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
36 $P4/mmm$	$7 mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	$7 mm2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1+c_1, 0, 2+2c_1\}\}$	
36 $P4/mmm$	$7 mm2_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	$7 mm2_z$	5 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	8 222 _d	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	8 222 _d	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	8 222 _d	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	8 222 _d	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	8 222 _d	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	9 $mm2_d$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	9 $mm2_d$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
36 $P4/mmm$	9 $mm2_d$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	10 $\bar{4}$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	10 $\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	10 $\bar{4}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	10 $\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	10 $\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	11 4	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
36 $P4/mmm$	11 4	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
36 $P4/mmm$	11 4	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	12 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	12 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	12 mmm	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	12 mmm	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	12 mmm	5 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
36 $P4/mmm$	12 mmm	6 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	12 mmm	7 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	12 mmm	8 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	13 mmm_d	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	13 mmm_d	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	13 mmm_d	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	13 mmm_d	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	13 mmm_d	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	14 $4/m$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	14 $4/m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	14 $4/m$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	14 $4/m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	14 $4/m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	15 422	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	15 422	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	15 422	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	15 422	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	15 422	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	16 $\bar{4}2m$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	16 $\bar{4}2m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	16 $\bar{4}2m$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
36 $P4/mmm$	$16 \bar{4}2m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	$16 \bar{4}2m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	$17 \bar{4}m2$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	$17 \bar{4}m2$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	$17 \bar{4}m2$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	$17 \bar{4}m2$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	$17 \bar{4}m2$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	$18 4mm$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	$18 4mm$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 2+2c_1\}\}$	
36 $P4/mmm$	$18 4mm$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
36 $P4/mmm$	$19 4/mmm$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	$19 4/mmm$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
36 $P4/mmm$	$19 4/mmm$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
36 $P4/mmm$	$19 4/mmm$	4 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
36 $P4/mmm$	$19 4/mmm$	5 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
37 $I4/mmm$	$2 \bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	$2 \bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	$2 \bar{1}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
37 $I4/mmm$	$2 \bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
37 $I4/mmm$	$3 2_z$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
37 $I4/mmm$	$3 2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	$3 2_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
37 $I4/mmm$	$3 2_z$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1, 3+2c_1, 4(1+c_1)\}\}$	
37 $I4/mmm$	$3 2_z$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
37 $I4/mmm$	$4 m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	$4 m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1+d_1, 1+d_2, 2+d_1+d_2\}\}$	22
37 $I4/mmm$	$4 m_z$	3 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
37 $I4/mmm$	$4 m_z$	4 $\{\{1,0,0\}, \{1,2,0\}, \{0,2,4\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
37 I4/mmm	4 m_z	5 $\{\{1,0,0\}, \{1,3,0\}, \{0,3,6\}\}$	
37 I4/mmm	4 m_z	6 $\{\{1,0,0\}, \{1,2+c_1,0\}, \{0,0,2+c_1\}\}$	
37 I4/mmm	4 m_z	7 $\{\{1,0,0\}, \{1,4+c_1,0\}, \{0,4+c_1,2(4+c_1)\}\}$	
37 I4/mmm	4 m_z	8 $\{\{1,0,0\}, \{1,2,0\}, \{0,2(2+d_1),2(3+d_1+d_2)\}\}$	24*
37 I4/mmm	4 m_z	9 $\{\{1,0,0\}, \{1,3,0\}, \{0,3(1+d_1),3(3+d_1+d_2)\}\}$	23*
37 I4/mmm	4 m_z	10 $\{\{1,0,0\}, \{1,3,0\}, \{0,3(2+d_1),3(3+d_1+d_2)\}\}$	24*
37 I4/mmm	4 m_z	11 $\{\{1,0,0\}, \{1,4+c_1,0\}, \{0,(4+c_1)(1+d_1),(4+c_1)(3+d_1+d_2)\}\}$	62*
37 I4/mmm	4 m_z	12 $\{\{1,0,0\}, \{1,4+c_1,0\}, \{0,(4+c_1)(2+d_1),(4+c_1)(3+d_1+d_2)\}\}$	63*
37 I4/mmm	5 $2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 I4/mmm	5 $2/m_z$	2 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
37 I4/mmm	5 $2/m_z$	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 I4/mmm	6 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
37 I4/mmm	6 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 I4/mmm	6 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 I4/mmm	6 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
37 I4/mmm	6 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 I4/mmm	6 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 I4/mmm	7 $mm2_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 I4/mmm	7 $mm2_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
37 I4/mmm	8 222 _d	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 I4/mmm	8 222 _d	2 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
37 I4/mmm	8 222 _d	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 I4/mmm	9 $mm2_d$	1 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
37 I4/mmm	9 $mm2_d$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 I4/mmm	9 $mm2_d$	3 $\{\{1,0,0\}, \{1,2,0\}, \{2,2,2(2+c_1)\}\}$	
37 I4/mmm	9 $mm2_d$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3+2c_1,3+2c_1,4(1+c_1)\}\}$	
37 I4/mmm	9 $mm2_d$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2+c_1\}\}$	
37 I4/mmm	10 $\bar{4}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
37 $I4/mmm$	$10\bar{4}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	$10\bar{4}$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	$10\bar{4}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
37 $I4/mmm$	$10\bar{4}$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	$10\bar{4}$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	11 4	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	11 4	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2 + c_1\}\}$	
37 $I4/mmm$	12 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	12 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	13 mmm_d	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	13 mmm_d	2 $\{\{1,0,0\}, \{1,2,0\}, \{0,0,2\}\}$	
37 $I4/mmm$	13 mmm_d	3 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	14 $4/m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	14 $4/m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	15 422	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	15 422	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	16 $\bar{4}2m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
37 $I4/mmm$	16 $\bar{4}2m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	16 $\bar{4}2m$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	16 $\bar{4}2m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
37 $I4/mmm$	16 $\bar{4}2m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	16 $\bar{4}2m$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	17 $\bar{4}m2$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	17 $\bar{4}m2$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	18 $4mm$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
37 $I4/mmm$	18 $4mm$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2 + c_1\}\}$	
37 $I4/mmm$	19 $4/mmm$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
37 $I4/mmm$	19 $4/mmm$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
38 $P\bar{3}$	2 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
38 $P\bar{3}$	2 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{2+2c_1, 2+2c_1, 3+3c_1\}\}$	
38 $P\bar{3}$	2 3	3 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 3+3c_1\}\}$	
38 $P\bar{3}$	2 3	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
39 $R\bar{3}$	2 3	1 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, c_1, 1+c_1\}\}$	
40 $P\bar{3}$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
40 $P\bar{3}$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
40 $P\bar{3}$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
40 $P\bar{3}$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
40 $P\bar{3}$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
40 $P\bar{3}$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{2+2c_1, 2+2c_1, 3+3c_1\}\}$	
40 $P\bar{3}$	3 3	3 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 3+3c_1\}\}$	
40 $P\bar{3}$	3 3	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
40 $P\bar{3}$	4 $\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
40 $P\bar{3}$	4 $\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
41 $R\bar{3}$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
41 $R\bar{3}$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
41 $R\bar{3}$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
41 $R\bar{3}$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
41 $R\bar{3}$	3 3	1 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, c_1, 1+c_1\}\}$	
41 $R\bar{3}$	4 $\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
41 $R\bar{3}$	4 $\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
42 $P\bar{3}12$	2 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
42 $P\bar{3}12$	2 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{2+2c_1, 2+2c_1, 3+3c_1\}\}$	
42 $P\bar{3}12$	2 3	3 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 3+3c_1\}\}$	
42 $P\bar{3}12$	2 3	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
42 $P\bar{3}12$	3 312	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
42 $P\bar{3}12$	3 312	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
43 P321	2 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
43 P321	2 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
43 P321	3 321	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
43 P321	3 321	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
43 P321	3 321	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
43 P321	3 321	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
44 R32	2 3	1 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, c_1, 1+c_1\}\}$	
44 R32	3 321	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
44 R32	3 321	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
45 P3m1	2 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
45 P3m1	2 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
45 P3m1	3 3m1	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
46 P31m	2 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
46 P31m	2 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{2+2c_1, 2+2c_1, 3+3c_1\}\}$	
46 P31m	2 3	3 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 3+3c_1\}\}$	
46 P31m	2 3	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
46 P31m	3 31m	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
46 P31m	3 31m	2 $\{\{1,0,0\}, \{0,1,0\}, \{2+2c_1, 2+2c_1, 3+3c_1\}\}$	
46 P31m	3 31m	3 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 3+3c_1\}\}$	
46 P31m	3 31m	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
47 R3m	2 3	1 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, c_1, 1+c_1\}\}$	
47 R3m	3 3m1	1 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, c_1, 1+c_1\}\}$	
48 P $\bar{3}$ 1m	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
48 P $\bar{3}$ 1m	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
48 P $\bar{3}$ 1m	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
48 P $\bar{3}$ 1m	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
48 P $\bar{3}$ 1m	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
48 P $\bar{3}$ 1m	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{2+2c_1, 2+2c_1, 3+3c_1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
48 $P\bar{3}1m$	3 3	3 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 3+3c_1\}\}$	
48 $P\bar{3}1m$	3 3	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
48 $P\bar{3}1m$	4 $\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
48 $P\bar{3}1m$	4 $\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
48 $P\bar{3}1m$	5 31m	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
48 $P\bar{3}1m$	5 31m	2 $\{\{1,0,0\}, \{0,1,0\}, \{2+2c_1, 2+2c_1, 3+3c_1\}\}$	
48 $P\bar{3}1m$	5 31m	3 $\{\{1,0,0\}, \{0,1,0\}, \{1+c_1, 1+c_1, 3+3c_1\}\}$	
48 $P\bar{3}1m$	5 31m	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
48 $P\bar{3}1m$	6 312	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
48 $P\bar{3}1m$	6 312	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
48 $P\bar{3}1m$	7 $\bar{3}1m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
48 $P\bar{3}1m$	7 $\bar{3}1m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
49 $P\bar{3}m1$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
49 $P\bar{3}m1$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
49 $P\bar{3}m1$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
49 $P\bar{3}m1$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
49 $P\bar{3}m1$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
49 $P\bar{3}m1$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
49 $P\bar{3}m1$	4 $\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
49 $P\bar{3}m1$	4 $\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
49 $P\bar{3}m1$	5 321	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
49 $P\bar{3}m1$	5 321	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
49 $P\bar{3}m1$	5 321	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
49 $P\bar{3}m1$	5 321	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
49 $P\bar{3}m1$	6 3m1	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
49 $P\bar{3}m1$	7 $\bar{3}m1$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
49 $P\bar{3}m1$	7 $\bar{3}m1$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
50 $R\bar{3}m$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
50 $R\bar{3}m$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
50 $R\bar{3}m$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
50 $R\bar{3}m$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
50 $R\bar{3}m$	3 3	1 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, c_1, 1+c_1\}\}$	
50 $R\bar{3}m$	4 $\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
50 $R\bar{3}m$	4 $\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
50 $R\bar{3}m$	5 321	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
50 $R\bar{3}m$	5 321	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
50 $R\bar{3}m$	6 3m1	1 $\{\{1,0,0\}, \{0,1,0\}, \{c_1, c_1, 1+c_1\}\}$	
50 $R\bar{3}m$	7 $\bar{3}m1$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
50 $R\bar{3}m$	7 $\bar{3}m1$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
51 $P\bar{6}$	2 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
51 $P\bar{6}$	2 2_z	2 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
51 $P\bar{6}$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
51 $P\bar{6}$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
51 $P\bar{6}$	4 6	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
52 $P\bar{6}$	2 m_z	1 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
52 $P\bar{6}$	2 m_z	2 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,1\}\}$	34
52 $P\bar{6}$	2 m_z	3 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
52 $P\bar{6}$	2 m_z	4 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,2\}\}$	34
52 $P\bar{6}$	2 m_z	5 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+2d_1), (1+c_1)(3+2d_1+d_2), 0\}, \{0,1,2\}\}$	59*
52 $P\bar{6}$	2 m_z	6 $\{\{1+c_1,0,0\}, \{2(1+c_1)(1+d_1), 2(1+c_1)(2+d_1+d_2), 0\}, \{1,0,2\}\}$	36*
52 $P\bar{6}$	2 m_z	7 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(4+d_1+2d_2), 0\}, \{1,1,2\}\}$	65*
52 $P\bar{6}$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
52 $P\bar{6}$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
52 $P\bar{6}$	4 $\bar{6}$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
52 $P\bar{6}$	4 $\bar{6}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
52 $P\bar{6}$	4 $\bar{6}$	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
52 $P\bar{6}$	4 $\bar{6}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
53 $P6/m$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
53 $P6/m$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
53 $P6/m$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
53 $P6/m$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
53 $P6/m$	3 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
53 $P6/m$	3 2_z	2 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
53 $P6/m$	4 m_z	1 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
53 $P6/m$	4 m_z	2 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,1\}\}$	34
53 $P6/m$	4 m_z	3 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
53 $P6/m$	4 m_z	4 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,2\}\}$	34
53 $P6/m$	4 m_z	5 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+2d_1), (1+c_1)(3+2d_1+d_2), 0\}, \{0,1,2\}\}$	59*
53 $P6/m$	4 m_z	6 $\{\{1+c_1,0,0\}, \{2(1+c_1)(1+d_1), 2(1+c_1)(2+d_1+d_2), 0\}, \{1,0,2\}\}$	36*
53 $P6/m$	4 m_z	7 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(4+d_1+2d_2), 0\}, \{1,1,2\}\}$	65*
53 $P6/m$	5 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
53 $P6/m$	5 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
53 $P6/m$	6 $2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
53 $P6/m$	6 $2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
53 $P6/m$	6 $2/m_z$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
53 $P6/m$	6 $2/m_z$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
53 $P6/m$	7 $\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
53 $P6/m$	7 $\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
53 $P6/m$	8 6	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
53 $P6/m$	9 $\bar{6}$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
53 $P6/m$	9 $\bar{6}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
53 $P6/m$	9 $\bar{6}$	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
53 $P6/m$	9 $\bar{6}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
53 $P6/m$	10 $6/m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
53 $P6/m$	10 $6/m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
54 $P622$	2 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
54 $P622$	2 2_z	2 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
54 $P622$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
54 $P622$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
54 $P622$	4 6	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
54 $P622$	5 321	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
54 $P622$	5 321	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
54 $P622$	5 321	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
54 $P622$	5 321	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
54 $P622$	6 312	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
54 $P622$	6 312	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
54 $P622$	7 622	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
54 $P622$	7 622	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
55 $P6mm$	2 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	2 2_z	2 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	4 6	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	5 31m	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	5 31m	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	6 3m1	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
55 $P6mm$	7 6mm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
56 $P\bar{6}m2$	2 m_z	1 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
56 $P\bar{6}m2$	2 m_z	2 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,1\}\}$	61
56 $P\bar{6}m2$	2 m_z	3 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
56 $P\bar{6}m2$	2 m_z	4 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,2\}\}$	61
56 $P\bar{6}m2$	2 m_z	5 $\{\{1+c_1,0,0\}, \{2(1+c_1)(1+d_1), 2(1+c_1)(2+d_1+d_2), 0\}, \{1,0,2\}\}$	60*

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
56 $P\bar{6}m2$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
56 $P\bar{6}m2$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
56 $P\bar{6}m2$	4 $\bar{6}$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
56 $P\bar{6}m2$	4 $\bar{6}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
56 $P\bar{6}m2$	4 $\bar{6}$	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
56 $P\bar{6}m2$	4 $\bar{6}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
56 $P\bar{6}m2$	5 312	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
56 $P\bar{6}m2$	5 312	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
56 $P\bar{6}m2$	6 3m1	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
56 $P\bar{6}m2$	7 $\bar{6}m2$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
56 $P\bar{6}m2$	7 $\bar{6}m2$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
57 $P\bar{6}2m$	2 m_z	1 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
57 $P\bar{6}2m$	2 m_z	2 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,1\}\}$	61
57 $P\bar{6}2m$	2 m_z	3 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
57 $P\bar{6}2m$	2 m_z	4 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,2\}\}$	61
57 $P\bar{6}2m$	2 m_z	5 $\{\{1+c_1,0,0\}, \{2(1+c_1)(1+d_1), 2(1+c_1)(2+d_1+d_2), 0\}, \{1,0,2\}\}$	60*
57 $P\bar{6}2m$	3 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
57 $P\bar{6}2m$	3 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
57 $P\bar{6}2m$	4 321	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
57 $P\bar{6}2m$	4 321	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
57 $P\bar{6}2m$	4 321	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
57 $P\bar{6}2m$	4 321	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
57 $P\bar{6}2m$	5 31m	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
57 $P\bar{6}2m$	5 31m	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
57 $P\bar{6}2m$	6 $\bar{6}$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
57 $P\bar{6}2m$	6 $\bar{6}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
57 $P\bar{6}2m$	6 $\bar{6}$	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
57 $P\bar{6}2m$	6 $\bar{6}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
57 $P\bar{6}2m$	7 $\bar{6}2m$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
57 $P\bar{6}2m$	7 $\bar{6}2m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
57 $P\bar{6}2m$	7 $\bar{6}2m$	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
57 $P\bar{6}2m$	7 $\bar{6}2m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	3 2_z	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	3 2_z	2 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	4 m_z	1 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	4 m_z	2 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,1\}\}$	61
58 $P6/mmm$	4 m_z	3 $\{\{1+c_1,0,0\}, \{0,1+c_1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	4 m_z	4 $\{\{1+c_1,0,0\}, \{(1+c_1)(1+d_1), (1+c_1)(2+d_1+d_2), 0\}, \{0,0,2\}\}$	61
58 $P6/mmm$	4 m_z	5 $\{\{1+c_1,0,0\}, \{2(1+c_1)(1+d_1), 2(1+c_1)(2+d_1+d_2), 0\}, \{1,0,2\}\}$	60*
58 $P6/mmm$	5 3	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	5 3	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	6 $2/m_z$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	6 $2/m_z$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	6 $2/m_z$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	6 $2/m_z$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	7 $\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	7 $\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	8 6	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	9 321	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	9 321	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	9 321	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	9 321	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
58 $P6/mmm$	10 $31m$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	10 $31m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	11 $\bar{6}$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	11 $\bar{6}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	11 $\bar{6}$	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	11 $\bar{6}$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	12 312	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	12 312	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	13 $3m1$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	14 $6/m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	14 $6/m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	15 $\bar{3}m1$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	15 $\bar{3}m1$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	16 622	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	16 622	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	17 $\bar{6}2m$	1 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	17 $\bar{6}2m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	17 $\bar{6}2m$	3 $\{\{1,0,0\}, \{2,3,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	17 $\bar{6}2m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	18 $\bar{3}1m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	18 $\bar{3}1m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	19 $6mm$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1+c_1\}\}$	
58 $P6/mmm$	20 $\bar{6}m2$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	20 $\bar{6}m2$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
58 $P6/mmm$	21 $6/mmm$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
58 $P6/mmm$	21 $6/mmm$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,2\}\}$	
59 $P23$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
59 $P23$	2 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	

Continued on next page

Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
59 $P23$	2 222	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
59 $P23$	2 222	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
59 $P23$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
59 $P23$	3 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
60 $F23$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
60 $F23$	2 222	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
60 $F23$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
61 $I23$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
61 $I23$	2 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
61 $I23$	2 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
61 $I23$	2 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
61 $I23$	2 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
61 $I23$	2 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
61 $I23$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
61 $I23$	3 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
61 $I23$	3 23	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
61 $I23$	3 23	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
61 $I23$	3 23	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
61 $I23$	3 23	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
62 $Pm\bar{3}$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
62 $Pm\bar{3}$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
62 $Pm\bar{3}$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
62 $Pm\bar{3}$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
62 $Pm\bar{3}$	3 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
62 $Pm\bar{3}$	3 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
62 $Pm\bar{3}$	3 222	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
62 $Pm\bar{3}$	3 222	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
62 $Pm\bar{3}$	4 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
62 $Pm\bar{3}$	4 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
62 $Pm\bar{3}$	4 mmm	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
62 $Pm\bar{3}$	4 mmm	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
62 $Pm\bar{3}$	5 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
62 $Pm\bar{3}$	5 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
62 $Pm\bar{3}$	6 $m\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
62 $Pm\bar{3}$	6 $m\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
63 $Fm\bar{3}$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
63 $Fm\bar{3}$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
63 $Fm\bar{3}$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
63 $Fm\bar{3}$	3 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
63 $Fm\bar{3}$	3 222	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
63 $Fm\bar{3}$	4 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
63 $Fm\bar{3}$	4 mmm	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
63 $Fm\bar{3}$	5 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
63 $Fm\bar{3}$	6 $m\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
64 $Im\bar{3}$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
64 $Im\bar{3}$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
64 $Im\bar{3}$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
64 $Im\bar{3}$	3 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
64 $Im\bar{3}$	3 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
64 $Im\bar{3}$	3 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
64 $Im\bar{3}$	3 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
64 $Im\bar{3}$	3 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
64 $Im\bar{3}$	3 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
64 $Im\bar{3}$	4 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
64 $Im\bar{3}$	4 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
64 $Im\bar{3}$	5 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
64 $Im\bar{3}$	5 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
64 $Im\bar{3}$	5 23	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
64 $Im\bar{3}$	5 23	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
64 $Im\bar{3}$	5 23	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
64 $Im\bar{3}$	5 23	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
64 $Im\bar{3}$	6 $m\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
64 $Im\bar{3}$	6 $m\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
65 $P432$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
65 $P432$	2 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
65 $P432$	2 222	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
65 $P432$	2 222	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
65 $P432$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
65 $P432$	3 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
65 $P432$	4 432	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
65 $P432$	4 432	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
66 $F432$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
66 $F432$	2 222	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
66 $F432$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
66 $F432$	4 432	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
67 $I432$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
67 $I432$	2 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
67 $I432$	2 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
67 $I432$	2 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
67 $I432$	2 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
67 $I432$	2 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
67 $I432$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
67 $I432$	3 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
67 $I432$	3 23	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
67 I432	3 23	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
67 I432	3 23	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
67 I432	3 23	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
67 I432	4 432	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
67 I432	4 432	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
68 P $\bar{4}3m$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
68 P $\bar{4}3m$	2 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
68 P $\bar{4}3m$	2 222	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
68 P $\bar{4}3m$	2 222	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
68 P $\bar{4}3m$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
68 P $\bar{4}3m$	3 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
68 P $\bar{4}3m$	4 $\bar{4}3m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
68 P $\bar{4}3m$	4 $\bar{4}3m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
69 F $\bar{4}3m$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
69 F $\bar{4}3m$	2 222	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
69 F $\bar{4}3m$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
69 F $\bar{4}3m$	4 $\bar{4}3m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
70 I $\bar{4}3m$	2 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
70 I $\bar{4}3m$	2 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
70 I $\bar{4}3m$	2 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
70 I $\bar{4}3m$	2 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
70 I $\bar{4}3m$	2 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
70 I $\bar{4}3m$	2 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
70 I $\bar{4}3m$	3 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
70 I $\bar{4}3m$	3 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
70 I $\bar{4}3m$	3 23	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
70 I $\bar{4}3m$	3 23	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
70 I $\bar{4}3m$	3 23	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
70 $I\bar{4}3m$	3 23	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
70 $I\bar{4}3m$	4 $\bar{4}3m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
70 $I\bar{4}3m$	4 $\bar{4}3m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
70 $I\bar{4}3m$	4 $\bar{4}3m$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
70 $I\bar{4}3m$	4 $\bar{4}3m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
70 $I\bar{4}3m$	4 $\bar{4}3m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
70 $I\bar{4}3m$	4 $\bar{4}3m$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
71 $Pm\bar{3}m$	2 $\bar{1}$	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
71 $Pm\bar{3}m$	2 $\bar{1}$	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
71 $Pm\bar{3}m$	3 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	3 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
71 $Pm\bar{3}m$	3 222	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
71 $Pm\bar{3}m$	3 222	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
71 $Pm\bar{3}m$	4 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	4 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
71 $Pm\bar{3}m$	4 mmm	3 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
71 $Pm\bar{3}m$	4 mmm	4 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
71 $Pm\bar{3}m$	5 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
71 $Pm\bar{3}m$	5 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	6 $m\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
71 $Pm\bar{3}m$	6 $m\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	7 432	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
71 $Pm\bar{3}m$	7 432	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	8 $\bar{4}3m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
71 $Pm\bar{3}m$	8 $\bar{4}3m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
71 $Pm\bar{3}m$	9 $m\bar{3}m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
71 $Pm\bar{3}m$	9 $m\bar{3}m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
72 $Fm\bar{3}m$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
72 $Fm\bar{3}m$	3 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	3 222	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
72 $Fm\bar{3}m$	4 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	4 mmm	2 $\{\{1,0,0\}, \{1,2,0\}, \{1,0,2\}\}$	
72 $Fm\bar{3}m$	5 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	6 $m\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	7 432	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	8 $\bar{4}3m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
72 $Fm\bar{3}m$	9 $m\bar{3}m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	2 $\bar{1}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	2 $\bar{1}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	2 $\bar{1}$	3 $\{\{2,0,0\}, \{0,2,0\}, \{0,0,2\}\}$	
73 $Im\bar{3}m$	3 222	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
73 $Im\bar{3}m$	3 222	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	3 222	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	3 222	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
73 $Im\bar{3}m$	3 222	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	3 222	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	4 mmm	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	4 mmm	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	5 23	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
73 $Im\bar{3}m$	5 23	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	5 23	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	5 23	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	

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Table A.1 – continued from previous page

ACC	P_N	B_N matrix row by row	c#
73 $Im\bar{3}m$	5 23	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	5 23	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	6 $m\bar{3}$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	6 $m\bar{3}$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	7 432	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	7 432	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	8 $\bar{4}3m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
73 $Im\bar{3}m$	8 $\bar{4}3m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	8 $\bar{4}3m$	3 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	8 $\bar{4}3m$	4 $\{\{1,0,0\}, \{0,1,0\}, \{3,3,4\}\}$	
73 $Im\bar{3}m$	8 $\bar{4}3m$	5 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	8 $\bar{4}3m$	6 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	
73 $Im\bar{3}m$	9 $m\bar{3}m$	1 $\{\{1,0,0\}, \{0,1,0\}, \{1,1,2\}\}$	
73 $Im\bar{3}m$	9 $m\bar{3}m$	2 $\{\{1,0,0\}, \{0,1,0\}, \{0,0,1\}\}$	

Table A.2 A list of extra conditions referenced in Table A.1. Each entry contains one or more rational polynomial functions that must simultaneously take on integer values. Furthermore, all variables are restricted to non-negative integer values, except for entries 26-29 where d_2 is further constrained by the inequalities presented and d_1 can be negative. Some of these conditions have no solutions; some have only a finite number of solutions, some have infinite families of solutions. A discussion of each of the solution space of each condition follows the table.

c#	extra conditions
1	$\frac{5+4d_1+d_1^2}{4+2d_1}$
2	$\frac{5+4d_1+d_1^2}{4+2d_1}$
3	$\frac{2d_1(1+d_1)}{1+d_1+d_2}$
4	$\frac{d_1(2+d_1)}{2+d_1+d_2}$
5	$\frac{2+2d_1+d_1^2}{2+d_1+d_2}$
6	$\frac{d_1(2+d_1)}{3+d_1+d_2}$
7	$\frac{2+2d_1+d_1^2}{3+d_1+d_2}$
8	$\frac{2(2+3d_1+d_1^2)}{3+d_1+d_2}$
9	$\frac{3+4d_1+d_1^2}{3+d_1+d_2}$
10	$\frac{5+4d_1+d_1^2}{3+d_1+d_2}$
11	$\frac{2(6+5d_1+d_1^2)}{3+d_1+d_2}$
12	$\frac{d_1(2+d_1)}{4+d_1+d_2}$
13	$\frac{2(2+3d_1+d_1^2)}{4+d_1+d_2}$
14	$\frac{3+4d_1+d_1^2}{4+d_1+d_2}$
15	$\frac{2(6+5d_1+d_1^2)}{4+d_1+d_2}$
16	$\frac{d_1(2+d_1)}{5+d_1+d_2}$
17	$\frac{3+4d_1+d_1^2}{5+d_1+d_2}$
18	$\frac{8+6d_1+d_1^2}{5+d_1+d_2}$

Continued on next page

Table A.2 – continued from previous page

c#	extra conditions	
19	$\frac{2d_1(1+d_1)}{3+2d_1+d_2}$	
20	$\frac{2(2+3d_1+d_1^2)}{4+2d_1+d_2}$	
21	$\frac{2(2+3d_1+d_1^2)}{5+2d_1+d_2}$	
22	$\frac{d_1(2+d_1)}{2+d_1+d_2}$	$\frac{2+2d_1+d_1^2}{2+d_1+d_2}$
23	$\frac{d_1(2+d_1)}{3+d_1+d_2}$	$\frac{2+2d_1+d_1^2}{3+d_1+d_2}$
24	$\frac{3+4d_1+d_1^2}{3+d_1+d_2}$	$\frac{5+4d_1+d_1^2}{3+d_1+d_2}$
25	$\frac{3+d_1}{6+2d_1+3d_2}$	$\frac{3+d_1}{3+d_1+d_2}$
26	$\frac{d_1(5+2d_1+3d_2)}{4+d_1+2d_2}$	$d_2 \geq \text{Max}[\frac{-1-2d_1}{2}, 0]$ d_1 can be negative
27	$\frac{d_1(7+2d_1+3d_2)}{4+d_1+2d_2}$	$d_2 \geq \text{Max}[\frac{-1-2d_1}{2}, 0]$ d_1 can be negative
28	$\frac{(1+d_1)(4+2d_1+3d_2)}{3+d_1+2d_2}$	$d_2 \geq \text{Max}[-d_1, 0]$ d_1 can be negative
29	$\frac{-2d_1^2+d_2-d_1(2+3d_2)}{3+d_1+2d_2}$	$d_2 \geq \text{Max}[-d_1, 0]$ d_1 can be negative
30	$\frac{2d_1(1+d_1)}{1+d_1+d_2}$	
31	$\frac{1+2d_1+2d_1^2}{1+d_1+d_2}$	
32	$\frac{2d_1(1+d_1)}{2+d_1+d_2}$	
33	$\frac{d_1(2+d_1)}{2+d_1+d_2}$	
34	$\frac{1+d_1+d_1^2}{2+d_1+d_2}$	
35	$\frac{2+2d_1+d_1^2}{2+d_1+d_2}$	
36	$\frac{3+6d_1+4d_1^2}{2(2+d_1+d_2)}$	
37	$\frac{2d_1(1+d_1)}{3+d_1+d_2}$	
38	$\frac{d_1(2+d_1)}{3+d_1+d_2}$	
39	$\frac{2+2d_1+d_1^2}{3+d_1+d_2}$	
40	$\frac{2(2+3d_1+d_1^2)}{3+d_1+d_2}$	

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Table A.2 – continued from previous page

c#	extra conditions	
41	$\frac{2(2+3d_1+d_1^2)}{3+d_1+d_2}$	
42	$\frac{3+4d_1+d_1^2}{3+d_1+d_2}$	
43	$\frac{5+4d_1+d_1^2}{3+d_1+d_2}$	
44	$\frac{2(6+5d_1+d_1^2)}{3+d_1+d_2}$	
45	$\frac{d_1(2+d_1)}{4+d_1+d_2}$	
46	$\frac{2(2+3d_1+d_1^2)}{4+d_1+d_2}$	
47	$\frac{3+4d_1+d_1^2}{4+d_1+d_2}$	
48	$\frac{2(6+5d_1+d_1^2)}{4+d_1+d_2}$	
49	$\frac{d_1(2+d_1)}{5+d_1+d_2}$	
50	$\frac{3+4d_1+d_1^2}{5+d_1+d_2}$	
51	$\frac{3+4d_1+d_1^2}{5+d_1+d_2}$	
52	$\frac{8+6d_1+d_1^2}{5+d_1+d_2}$	
53	$\frac{1+2d_1+2d_1^2}{2+2d_1+d_2}$	
54	$\frac{2d_1(1+d_1)}{3+2d_1+d_2}$	
55	$\frac{3+8d_1+4d_1^2}{3+2d_1+d_2}$	
56	$\frac{2(2+3d_1+d_1^2)}{4+2d_1+d_2}$	
57	$\frac{2(2+3d_1+d_1^2)}{4+2d_1+d_2}$	
58	$\frac{4d_1(1+d_1)}{3+2d_1+2d_2}$	
59	$\frac{1+2d_1+4d_1^2}{6+4d_1+2d_2}$	
60	$\frac{2d_1(1+d_1)}{2+d_1+d_2}$	$\frac{3+6d_1+4d_1^2}{2(2+d_1+d_2)}$
61	$\frac{1-d_1^2}{2+d_1+d_2}$	$\frac{1+d_1+d_1^2}{2+d_1+d_2}$
62	$\frac{d_1(2+d_1)}{3+d_1+d_2}$	$\frac{2+2d_1+d_1^2}{3+d_1+d_2}$

Continued on next page

Table A.2 – continued from previous page

c#	extra conditions		
63	$\frac{3+4d_1+d_1^2}{3+d_1+d_2}$	$\frac{5+4d_1+d_1^2}{3+d_1+d_2}$	
64	$\frac{1+d_1^2}{3+d_1+2d_2}$	$\frac{1+d_2+d_1(2+d_2)}{3+d_1+2d_2}$	
65	$\frac{1+d_1+d_1^2}{4+d_1+2d_2}$	$\frac{3+2d_2+2d_1(2+d_2)}{2(4+d_1+2d_2)}$	
66	$\frac{1-d_1^2}{1+d_1+2d_2}$	$\frac{(-1+d_1)d_2}{1+d_1+2d_2}$	$\frac{(1+d_1)(1+d_2)}{1+d_1+2d_2}$
67	$\frac{2(2+d_1)d_2(1+d_2)}{3+d_1+2d_2+d_1d_2+d_3}$	$\frac{2(3+d_1+2d_2+d_1d_2+d_3)}{2+d_1}$	
68	$\frac{(1+d_1)(3+8d_2+4d_2^2)}{4+2d_2+d_1(3+2d_2)+d_3}$	$\frac{4+3d_1+2d_2+2d_1d_2+d_3}{1+d_1}$	
69	$\frac{2(1+d_1)(1+d_3)}{7+4d_3+d_2(2+d_3)+d_1(3+2d_3)}$	$\frac{2(1+d_1)}{4+2d_1+d_2}$	
70	$\frac{2(2+d_1)(1+d_3)}{8+5d_3+d_2(2+d_3)+d_1(3+2d_3)}$	$\frac{2(2+d_1)}{5+2d_1+d_2}$	
71	$\frac{2(3+d_1)(1+d_3)}{9+6d_3+d_2(2+d_3)+d_1(3+2d_3)}$	$\frac{2(3+d_1)}{6+2d_1+d_2}$	
72	$\frac{(1+d_1)(1+2d_3)}{5+4d_3+2d_1(1+d_3)+d_2(3+2d_3)}$	$\frac{1+d_1}{2+d_1+d_2}$	
73	$\frac{(2+d_1)(1+2d_3)}{7+6d_3+2d_1(1+d_3)+d_2(3+2d_3)}$	$\frac{2+d_1}{3+d_1+d_2}$	
74	$\frac{(3+d_1)(3+2d_3)}{6(2+d_3)+2d_1(2+d_3)+d_2(5+2d_3)}$	$\frac{3+d_1}{3+d_1+d_2}$	

For each c# that is not specifically listed in the paragraphs below, there are infinitely many solutions. Each of these cases has a single quotient of polynomials of the form $\frac{f(d_1)}{g(d_1)+d_2}$, where the polynomial coefficients are all positive integers, and the variables d_1 and d_2 must be non-negative integers, and $g(d_1) \neq 0$. Thus, the integer value k of the quotient must be positive. Solving for d_2 in terms of k , we obtain $d_2 = \frac{f(d_1)}{k} - g(d_1)$. For a given d_1 , every integer value of $k > 0$ that divides $f(d_1)$ provides an integer solution for d_2 . For any d_1 , $k = f(d_1)$ will always be a solution; but there will usually be others as well. Because d_1 has infinite range, the condition has an infinite number of solutions.

c# 1 and 2:

There are no solutions. To illustrate this, we can expand the quotient as $1 + \frac{d_1}{2} + \frac{1}{2(2+d_1)}$. Since $\frac{d_1}{2}$ is a half-integer and $0 < \frac{1}{2(2+d_1)} < \frac{1}{2}$, the sum cannot be integral.

c# 22:

There is only one solution. Since both quotients must be integers, it follows that their difference must also be an integer. If we subtract the first quotient from the second, it yields $\frac{2}{2+d_1+d_2}$ which is only an integer when $d_1 = d_2 = 0$.

c# 23, 24, 62, and 63:

There are no solutions. If we take the difference of the two quotients, we get $\frac{2}{3+d_1+d_2}$ which must lie strictly between 0 and 1, and therefore cannot be an integer.

c# 25:

There are no solutions. By observation, the second quotient is positive but less than or equal to 1 with equality only when $d_2 = 0$. However, replacing d_2 with 0 reduces the first quotient to $\frac{1}{2}$ which is clearly not an integer.

c# 36, 59, 60, and 65:

There are no solutions. These cases contain a quotient where the numerator is odd while the denominator is even; thus, it can never be an integer.

c# 58:

There is one infinite one-dimensional family of solutions. Clearly, $d_1 = 0$ is a solution for any $d_2 \geq 0$. If $d_1 \neq 0$, then the numerator of the quotient is even while the denominator is odd, so the

quotient cannot be integral.

c# 61:

There is only one solution. If we take the sum of the two quotients, we get $\frac{2+d_1}{2+d_1+d_2}$ which will only be an integer if $d_2 = 0$. With this in mind we can rewrite the first quotient as $\frac{1-d_1^2}{2+d_1} = 2 - d_1 - \frac{3}{2+d_1}$ which is only integral if $d_1 = 1$. Thus, the only solution for this case is $d_1 = 1$ and $d_2 = 0$.

c# 69, 70, 72, and 73:

There are no solutions. The second quotient in each case has a denominator that is strictly greater than the non-zero numerator and thus it cannot be an integer.

c# 71 and 74:

There are no solutions. The second quotient in each case has a denominator that is d_2 greater than the numerator, so that it is integral if and only if $d_2 = 0$. However, applying $d_2 = 0$ to the first quotient makes its denominator $3 + d_1$ greater than its numerator, so that the first quotient is not an integer.

c# 26, 27, 28, 29, 64, 66, 67, and 68:

There are infinitely many solutions. These cases are more complicated and are still under investigation.