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On the classification and enumeration of the irreducible co-representations of magnetic space groups

Maia N Angelova† and L L Boyle‡

† Oxford University Department of Physics, Theoretical Physics, 1, Keble Road, Oxford OX1 3NP, UK

‡ University Chemical Laboratory, Canterbury, Kent CT2 7NH, UK

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Abstract. A generalization of Wintgen's method for classifying space-group representations is made to enable the infinite set of co-representations of magnetic space groups to be classified and enumerated. Using this method, all special points, lines and planes in the Brillouin zone model for magnetic crystals are identified. Arithmetic crystal-classes of magnetic space groups are introduced, fully listed and used to classify magnetic space groups and their co-representations. A version of Burnside's theorem adapted to co-representations is constructed and used to solve completely the enumeration problem of co-representations of magnetic space groups.

1. Introduction

The aim of this paper is to present a systematic way of classifying and enumerating the irreducible co-representations of magnetic space groups. These groups [1, 2], which contain both unitary and anti-unitary operations, describe the symmetry of paramagnetic crystals and also a large class of magnetically-ordered crystals. As abstract groups isomorphic to space groups, magnetic space groups do have irreducible representations but these are not themselves relevant to most physical applications since wavefunctions in magnetic crystals transform as co-representations [3] rather than as ordinary, linear representations. As in the case of the irreducible representations of ordinary space groups, the irreducible co-representations of magnetic space groups are constructed by induction from the irreducible representations of the invariant (or normal) subgroup of three-dimensional translations. This translational group is an Abelian group and its irreducible representations are exponentials of the type $e^{2\pi i \boldsymbol{k}\cdot\boldsymbol{t}}$ defined by three parameters, $\{p, q, r\}$, which can be regarded as the components of a wave vector $\boldsymbol{k} = (p, q, r)$ in the reciprocal space. The other vector, $\boldsymbol{t} = (v_x, v_y, v_z)$, is the vector of pure translations with integer components v_x, v_y, v_z and is defined in the real (direct) space. The translational group is of infinite order and hence the irreducible representations and co-representations of the space groups are infinite in number yet they may be classified into a finite number of strata of inequivalent translational types. With the exception of the trivial case of the invariant strata, the strata are to be regarded as infinite sets of irreducible representations any one of which can be specified by choosing specific values for any parameters (p, q, r) associated with the stratum. There are four types of translational strata of irreducible representations. The *invariant* strata are discrete, finite in number and correspond to special points in the Brillouin zone model. The *univariant* strata depend on one parameter and correspond to lines of special points. The *divariant* strata depend on two parameters and correspond to planes while the single *trivariant* stratum depends on three parameters and corresponds to all general points in the Brillouin zone model. The range of each parameter is finite and may be broken when special values exist. In such cases the irreducible representation splits into a sum of irreducible representations of lower dimensions which belong to strata specified by fewer parameters (i.e. have fewer 'degrees of freedom'). The individual representations are 'full-group representations' and would be constructed from the 'little-group representations' of the Brillouin zone model by constructing an orbit (or 'star') of equivalent wave vectors $\boldsymbol{k}$. The orbit containing the star of the wave vector $\boldsymbol{k}$ contains the little-group representation $e^{2\pi i \boldsymbol{k}\cdot\boldsymbol{t}}$ and all representations $e^{2\pi i \boldsymbol{k}'\cdot\boldsymbol{t}}$ characterized by different wave vectors $\boldsymbol{k}'$ (known as 'rays' in the star) satisfying the condition $\boldsymbol{k}' = R_i\boldsymbol{k}$ where R_i is a point-group operation of the space group.

The problem of the classification and enumeration of the translational strata of the irreducible representations of 230 classical space groups was solved by Wintgen [4] and the resulting principles were used by Slater [5] in his presentation of parts of the little-group character tables of 20 important space groups. Wintgen's contribution was to recognize that the problem of finding all such strata in a three-dimensional reciprocal space was isomorphic to the direct-space problem started by Niggli [6] and solved completely by Wyckoff [7] who found all strata of sets of inequivalent points for every space group. In reciprocal space, Jan [8] studied the symmetries of Fermi surfaces while Aroyo and Wondratschek [9] recently considered the asymmetric units geometrically.

The essence of Wintgen's method is that the space used to classify the orbits of irreducible representations was not necessarily isomorphic to that of the space group being studied. The space group used to classify the translational strata became known as the 'reciprocal space group' which was in only 47 cases isomorphic to the original space group. The reciprocal space group has the property of always belonging to one of the 73 types of symmorphic space groups, i.e. one of those space-group types which contain no free elements other than pure translations. In three-dimensional space, each arithmetic crystal-class [10] contains only one symmorphic space group and hence these 73 symmorphic space groups may be used to characterize the classes.

The problem of the classification of space-group representations into translational strata is one which depends on the arithmetic crystal-class to which the space group belongs. Confusion has been caused in the literature by regarding it as a problem which depends on the arithmetic crystal-class characterizing the holomorph of the crystal system yet having the same lattice. This approach underlies the notation introduced by Bouckaert *et al* [11] which has now become standard for the labelling of translational strata of space-group representations. Wintgen's work was not, however, used in some extensive computations of little-group character tables [12, 13] nor in associated work [14]. These tables suffer from omissions (divariant and trivariant strata and occasionally certain invariant strata are not included) and also have extraneous entries (parts of univariant or divariant strata are listed as invariant strata for non-special values of the parameters) as explained by Boyle [15].

In this paper we generalize Wintgen's method to magnetic space groups by introducing in section 2 an auxiliary non-magnetic space group which allows one to classify the irreducible co-representations and identify the symmetry points in the Brillouin zone of magnetic crystals. The classification of space-group co-representations depends on the arithmetic crystal-class of magnetic space groups which we define in section 3. A complete list of such classes for all magnetic space-group types is given. In section 4 we consider the problem of enumerating the irreducible co-representations within a given translational stratum and present a new extension of a theorem of Burnside which enables it to be applied to co-representations. Together with the generalization of Wintgen's method, the extension of Burnside's theorem enables one to solve completely the problem of the classification and enumeration of the irreducible co-representations of magnetic space groups. The important aspects of the theory are illustrated by the examples given in section 5.

The term 'co-representations' in this paper will always be taken to mean 'full-group co-representations' and never 'little-group co-representations' [16, 17].

2. Classification of the co-representations of magnetic space groups

A magnetic space group M contains a halving non-magnetic subgroup H of unitary spatial-symmetry operations, $u_i \in H$ $(i = 1, 2, \ldots, |H|)$, where $|H|$ is the order of the group H. We may write $M = H + a_0 H$ where the factor $a_0 = \theta u' = u'\theta$ is a product of time inversion θ [18] with a spatial operation u'. It is well known that θ commutes with all spatial operations.

As an abstract group, M is isomorphic to a non-magnetic group G. The operation u' is the identity when M is a 'grey' group, i.e. $M = H + \theta H$, but belongs to the coset $(G - H)$ when M is a 'black-and-white' group, i.e. $M = H + \theta(G - H)$.

According to a theorem of Hermann [19], the space group H must be either a *zellengleiche* [19] (or *translationengleiche* [20]) or a *klassengleiche* subgroup of G. We shall accordingly refer to the magnetic space group M as being *zellengleich* or *klassengleich* depending on the type of halving subgroup H.

The operation of time inversion, θ, is anti-unitary as also are the factor a_0 and all elements belonging to the coset $a_0 H$. Such elements cause complex conjugation of the wavefunctions and consequently the latter transform as co-representations rather than as ordinary linear representations in magnetic crystals where the symmetry is described by a magnetic group.

Co-representations were introduced in physics by Wigner [3]. They can be defined in terms of a set of matrices, $\mathcal{D} = \{D(u_i), D(a_i) \mid u_i \in H, a_i \in a_0 H\}$, which satisfy a generalized homomorphism rule of the type

$$D(g_1)D(g_2)^{g_1} = D(g_1 g_2) \qquad \forall g_1, g_2 \in M \tag{1}$$

for all elements g_i $(i = 1, 2, \ldots, |M|)$ of the group M. The superscript g_1 only implies complex conjugation when g_1 is an anti-unitary operation, i.e. $g_1 \in a_0 H$, but not when g_1 is a unitary operation, i.e. $g_1 \in H$. Equation (1) also shows that co-representations are a particular type of the semi-linear representations originally defined by Nakayama and Shoda [21].

Wigner [3] suggested a method for constructing irreducible co-representations by induction from the irreducible representations, $\Delta = \{\Delta(u_i) \mid u_i \in H, i = 1, 2, \ldots, |H|\}$, of the halving non-magnetic subgroup H into M. He also classified the irreducible co-representations as belonging to types a, b or c which can be determined using Dimmock and Wheeler's character test [22].

For a magnetic space group M, the infinite set of irreducible co-representations can be further classified into inequivalent translational strata by constructing orbits of the translational representations $e^{2\pi i \boldsymbol{k}\cdot\boldsymbol{t}}$ in M. These orbits may be superorbits of those in the halving space group H due to the Wigner induction described above.

2.1. Auxiliary space group

The construction of translational strata of co-representations of the magnetic group involves a procedure similar to that used in the corresponding construction for representations of an ordinary space group but includes the effect of both the unitary point-group generators and the anti-unitary factor a_0. The effect of unitary operations is the same as in the ordinary space group and is well known, while the effect of the anti-unitary factor $a_0 = u'\theta$ may be regarded as time inversion θ which produces complex conjugation of the exponential function followed by the unitary generator u':

$$a_0 \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{t}} = (u'\theta)\mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{t}} = u'\mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{t}} = u'\mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\cdot(-\boldsymbol{t})}. \tag{2}$$

Time inversion is therefore tantamount to any operation which reverses the sign of the translational vector $\boldsymbol{t}$ in direct space and is, therefore, in this particular problem, equivalent to that of space inversion in the origin, $\{S_2|000\} \equiv \{\bar{x}\bar{y}\bar{z}|000\}$, i.e.

$$\theta \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{t}} \simeq \{S_2|000\}\mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{t}}. \tag{3}$$

The orbits of irreducible co-representations of magnetic space groups are therefore identical to the orbits of the irreducible representations of a non-magnetic auxiliary space group A which can be constructed for any magnetic group M by replacing the time inversion by space inversion in the origin wherever it appears as a factor in the element of the magnetic group.

In the case of grey groups,

$$A \simeq \begin{cases} H + \{S_2|000\}H & \text{when } H \text{ is non-centrosymmetric} \\ H & \text{when } H \text{ already contains a centre of symmetry.} \end{cases} \tag{4}$$

In the case of *zellengleichen* black-and-white groups, replacement of θ by $\{S_2|000\}$ gives

$$A \simeq \begin{cases} H + \{S_2|000\}(G - H) & \text{when both } G \text{ and } H \text{ are non-centrosymmetric} \\ H & \text{when } G \text{ but not } H \text{ is centrosymmetric} \\ G & \text{when both } G \text{ and } H \text{ are centrosymmetric.} \end{cases} \tag{5}$$

In the case of *klassengleichen* black-and-white groups, replacement of θ by $\{S_2|000\}$ gives

$$A \simeq \begin{cases} H + \{S_2|000\}(G - H) & \text{when both } G \text{ and } H \text{ are non-centrosymmetric} \\ H & \text{when both } G \text{ and } H \text{ are centrosymmetric.} \end{cases} \tag{6}$$

Equations (4)–(6) clearly show that the auxiliary space group A contains space inversion for all grey groups, all *klassengleichen* black-and-white groups and for those *zellengleichen* black-and-white groups with centrosymmetric subgroup H.

Then, following Wintgen [4], we determine the reciprocal space group R of the auxiliary group A. R is always isomorphic to one of the 73 symmorphic space-group types. The strata of Wyckoff sets of points of the reciprocal group R are precisely those required for determining the inequivalent translational strata of both the irreducible representations of the non-magnetic group A and the irreducible co-representations of the magnetic group M. We have used the Wyckoff sets of points which are listed in the various editions of *International Tables* [23, 24, 20] to determine the inequivalent orbits of irreducible co-representations for all 1421 magnetic space groups. Comparison of our results with the corresponding little-group results published in the tables of Miller and Love [12] yields a complete explanation of their systems of notation and indicates which co-representations were omitted by them and which were included more than once albeit under different names. Typical examples are given in section 5.

The reciprocal space groups R of all magnetic space groups M are listed in section 3. Since the reciprocal group of a group containing space inversion is centrosymmetric itself, R is always centrosymmetric for grey groups and *klassengleichen* black-and-white groups, while for 49 classes of *zellengleichen* black-and-white symmetries R does not contain the space inversion. This latter result is in full agreement with Cracknell [25, 26] who, when studying the symmetry of the energy functions in magnetic crystals, also found that they are described by symmorphic, non-magnetic groups and listed the 49 cases where there is no centre of symmetry.

2.2. Special symmetries in the Brillouin zones of magnetic crystals

A traditional approach to the discussion of energies and wavefunctions in crystals has involved the first Brillouin zone [27] which is a primitive unit cell of the reciprocal space. It is usually constructed in a way similar to the Wigner–Seitz cell of direct space, i.e. by choosing as origin any one of the lattice points and drawing the planes that perpendicularly bisect the lines joining this point to its nearest neighbours. It contains the wave vector $\boldsymbol{k} = 0$ and all wave vectors $\boldsymbol{k}$ and $-\boldsymbol{k}$ which satisfy the equations of planes defining its boundaries, $\boldsymbol{k} \cdot \boldsymbol{g}_i = \frac{1}{2}\boldsymbol{g}_i \cdot \boldsymbol{g}_i$, where the $\boldsymbol{g}_i$ $(i = 1, 2, 3)$ are the reciprocal-lattice vectors. The advantage of choosing the Wigner–Seitz cell is that its centre ($\boldsymbol{k} = 0$) necessarily possesses the full point-group symmetry of the reciprocal lattice. However, for crystals belonging to low-symmetry (i.e. triclinic and monoclinic) crystal systems, the geometrical construction of the Wigner–Seitz unit cell of reciprocal space is usually exceedingly tedious and this cell is replaced by a parallelepiped constructed using the reciprocal-lattice vectors $\boldsymbol{g}_i$ [17].

Whichever unit cell is chosen, point symmetries within the lattice are limited by the actual point group and not by the holosymmetric point group of the reciprocal lattice, as has often been considered in the literature [12]. It should be remembered that whereas in direct space there are 230 types of space groups which are relevant to non-magnetic crystals, only 73 of these, namely the symmorphic groups, are also relevant to physical applications of the reciprocal space.

Because the reciprocal lattice is discrete, there are in principle special points, lines and planes where the local (or site) symmetry is higher than that of immediately adjacent points. We shall refer to these points as having ‘special symmetries’ while points which have only translational symmetry are known as ‘general points’. The significance of the existence of special points, lines and planes is that they provide a basis for classifying translational symmetries in direct space and hence a basis for classifying the translational strata of irreducible representations of the space group. What is even more important for quantum-mechanical applications is that the special symmetries provide a classification scheme for eigenfunctions and energies.

All inequivalent special symmetries in the first Brillouin zone of non-magnetic crystals can easily be found using Wintgen’s method. All we need to do is to identify the reciprocal space group R of the space group under consideration. The Wyckoff sets of points of R will describe precisely the special points, lines and planes in the Brillouin zone. The latter are, however, labelled by using an appropriate extension of the standard notation introduced in [11].

The Brillouin zone of magnetic crystals can be constructed geometrically using the reciprocal-lattice vectors $\boldsymbol{g}_i$ $(i = 1, 2, 3)$, defined by Gibbs’ formulae. These are derived from the lattice vectors of the magnetic unit cell in the real space. Instructive examples of such geometrical constructions are given in [17]. Account needs to be taken of those anti-ferromagnetic crystals where the unit cell is of black-and-white type [29, 30] in which case a basic translation is doubled. Hence one or more reciprocal-lattice vectors can be shorter and the size and shape of the Brillouin zone may change when the crystal passes from a paramagnetic to an anti-ferromagnetic phase.

However, the concept of the common reciprocal space group R allows us to choose the Brillouin zone of a magnetic space group M to be isomorphic to the Brillouin zone of the auxiliary non-magnetic group A. The main advantage of this approach is that we use Brillouin zones which are already well known and their special symmetries are well identified by the Wyckoff sets of points of R.

From equations (4)–(6) and associated discussion it is clear that the Brillouin zone needed to describe the translational symmetry of the magnetic group M will always be that of a centrosymmetric space group unless the halving non-magnetic group H is non-centrosymmetric and/or the coset $(G - H)$ does not contain any purely translational operations. In section 5 an example of a suitable choice of a Brillouin zone for the anti-ferromagnetic phase of solid oxygen is given.

3. Arithmetic crystal-classes of magnetic space groups

Arithmetic crystal-classes form the basis for classifying space groups. To provide a formal definition one considers the automorphism group, $GL(3, \mathbb{Z})$, of the three-dimensional translation group relevant to a lattice having an origin which is left invariant by the automorphisms. This group has an infinite number of finite subgroups which belong to 73 conjugacy classes. A space group is describable as an extension of its normal Abelian subgroup of translations by a finite subgroup of $GL(3, \mathbb{Z})$. The details of the composition of the elements in terms of the automorphism (point-group part) and a translation are determined by the cohomology of the extension. All space groups generated using a finite automorphism group from a given conjugacy class of subgroups of $GL(3, \mathbb{Z})$ are said to belong to the same arithmetic crystal-class.

In practice, it is simpler to consider an arithmetic crystal-class of space groups as consisting of all space groups having the same geometric crystal-class (or point group), the same lattice and the same setting of the point-group parts of the symmetry elements with respect to that lattice. This definition will now be applied to both non-magnetic and magnetic space groups. As already mentioned, each arithmetic crystal-class of three-dimensional crystallographic space groups contains just one symmorphic space group. This latter group is used to characterize the class and hence there are 73 arithmetic crystal-classes for the 230 crystallographic space-group types.

A formal definition of a magnetic arithmetic crystal-class can be constructed by considering all the different possible conjugacy classes of finite subgroups of the automorphism groups of the three-dimensional magnetic translation groups. These automorphism groups were identified by Janner [28] as subgroups of index 7 of $GL(3, \mathbb{Z})$ in the case of the *klassengleichen* magnetic groups and $GL(3, \mathbb{Z})$ itself in the case of the *zellengleichen* magnetic groups. The construction of the magnetic space groups then follows in a manner similar to that described for the ordinary space groups. In a simpler approach, we recognize that there are significant differences in both the geometric crystal-classes and the lattices. Compared with the 32 geometric crystal-classes of ordinary crystallographic point groups, there are 90 geometric crystal-classes of magnetic point groups made up of 32 grey and 58 black-and-white point groups. There are 36 types of magnetic lattices of which 14 coincide with the ordinary Bravais lattice-types while the other 22 are black-and-white types, i.e. the generators include a black-and-white non-primitive translation. The full list of magnetic lattices was produced by Belov *et al* [29, 30] whose notation will be used to distinguish between the black-and-white lattices. In this system a capital letter without a subscript denotes a Bravais lattice-type while a capital letter with a subscript denotes one of the black-and-white lattice-types. The role of the subscript is to give information about the coloured translation. Thus the unit cell of the monoclinic black-and-white lattice P_b is based on that of the primitive monoclinic lattice, P, with white points at the apices but, in addition, black points at the midpoints of those edges parallel to the twofold axis.

Each arithmetic crystal-class of magnetic space groups consists of all magnetic space groups having the same geometric magnetic crystal-class, the same magnetic lattice and an equivalent setting of the point-group parts of the symmetry elements with respect to that lattice. We have thus classified all 1191 black-and-white and 230 grey magnetic space-group types into 331 magnetic arithmetic crystal-classes. In detail, the 674 *zellengleichen* dichromatic groups belong to 148 magnetic arithmetic crystal-classes while the 517 *klassengleichen* dichromatic groups belong to 110 such classes. Like the 230 ordinary space groups, the 230 grey groups belong to 73 arithmetic crystal-classes but unlike the ordinary groups these magnetic arithmetic crystal-classes only correspond to the 24 centrosymmetric reciprocal space groups. The complete list of arithmetic crystal-classes of non-magnetic and magnetic space groups is presented in tables 1–7.

Table 1. Arithmetic crystal-classes of triclinic space groups.

Reciprocal space group	Non-magnetic arithmetic crystal-classes	Magnetic arithmetic crystal-classes
$P1 \equiv C_1^1$	$1P \equiv \{C_1^1\}$	$\bar{1}'P$
$P\bar{1} \equiv S_2^1$	$\bar{1}P \equiv \{S_2^1\}$	$1P_s, \bar{1}P_s, 1'P, \bar{1}1'P$

Table 2. Arithmetic crystal-classes of monoclinic space groups.

Reciprocal space group	Non-magnetic arithmetic crystal-classes	Magnetic arithmetic crystal-classes
$P2 \equiv C_2^1$	$2P \equiv \{C_2^{1,2}\}$	$m'P, 2/m'P$
$C2 \equiv C_2^3$	$2C \equiv \{C_2^3\}$	$m'C, 2/m'C$
$Pm \equiv C_{1h}^1$	$mP \equiv \{C_{1h}^{1,2}\}$	$2'P, 2'/mP$
$Cm \equiv C_{1h}^3$	$mC \equiv \{C_{1h}^{3,4}\}$	$2'C, 2'/mC$
$P2/m \equiv C_{2h}^1$	$2/mP \equiv \{C_{2h}^{1,2,4,5}\}$	$\left\{\begin{array}{l} 2'/m'P, 2P_a, 2P_b, 2P_C, mP_a, mP_b, mP_C, \\ 2/mP_a, 2/mP_b, 2/mP_C, 21'P, m1'P, 2/m1'P \end{array}\right.$
$C2/m \equiv C_{2h}^3$	$2/mC \equiv \{C_{2h}^{3,6}\}$	$\left\{\begin{array}{l} 2'/m'C, 2C_c, 2C_a, mC_c, mC_a, 2/mC_c, 2/mC_a, \\ 21'C, m1'C, 2/m1'C \end{array}\right.$

To determine the magnetic arithmetic crystal-class we use rules similar to those applied to crystallographic space groups [20]. The differences are due to the coloured generators (identifiable by the occurrence of a prime in the Hermann–Mauguin-type symbol for the magnetic group) and to the coloured lattice-type (identifiable by the presence of a subscript to the capital letter denoting the centring type of the Bravais lattice). For example the black-and-white group $C_{2h}^5(C_2^2) \equiv P2_1/c'$ belongs to the magnetic arithmetic class $2/m'P$, the group $C_2^1(C_2^2) \equiv P_b2_1$ belongs to the class $2P_b$ while the group $C_2^1(C_2^1) \equiv P_a2$ belongs to the class $2P_a$.

Table 3. Arithmetic crystal-classes of orthombic space groups.

Reciprocal space group	Non-magnetic arithmetic crystal-classes	Magnetic arithmetic crystal-classes
$P222 \equiv D_2^1$	$222P \equiv \{D_2^{1-4}\}$	$m'm'2P, m'm'm'P$
$C222 \equiv D_2^6$	$222C \equiv \{D_2^{5,6}\}$	$m'm'2C, m'm'm'C, m'm'2A$
$F222 \equiv D_2^7$	$222I \equiv \{D_2^{8,9}\}$	$m'm'2I, m'm'm'I$
$I222 \equiv D_2^8$	$222F \equiv \{D_2^7\}$	$m'm'2F, m'm'm'F$
$Pmm2 \equiv C_{2v}^1$	$mm2P \equiv \{C_{2v}^{1-10}\}$	$2'2'2P, m'm2'P, m'mmP$
$Cmm2 \equiv C_{2v}^{11}$	$mm2C \equiv \{C_{2v}^{11-13}\}$	$2'2'2C, mmm'C, m'm2'A$
$Amm2 \equiv C_{2v}^{14}$	$mm2A \equiv \{C_{2v}^{14-17}\}$	$22'2'C, m'm2'C, m'mmC, mm'2'A$
$Fmm2 \equiv C_{2v}^{18}$	$mm2I \equiv \{C_{2v}^{20-22}\}$	$2'2'2I, m'm2'I, m'mmI$
$Imm2 \equiv C_{2v}^{20}$	$mm2F \equiv \{C_{2v}^{18,19}\}$	$2'2'2F, m'm2'F, m'mmF$
$Pmmm \equiv D_{2h}^1$	$mmmP \equiv \{D_{2h}^{1-16}\}$	$\begin{cases} m'm'mP, 222P_a, 222P_C, 222P_I, \\ mm2P_c, mm2P_a, mm2P_C, mm2P_A, mm2P_I, \\ mmmP_a, mmmP_C, mmmP_I, \\ 2221'P, mm21'P, mmm1'P. \end{cases}$
$Cmmm \equiv D_{2h}^{19}$	$mmmC \equiv \{D_{2h}^{17-22}\}$	$\begin{cases} m'm'mC, mm'm'C, 222C_c, 222C_a, 222C_A, \\ mm2C_c, mm2C_a, mm2C_A, mm2A_a, mm2A_c, \\ mm2A_C, mmmC_c, mmmC_a, mmmC_A, \\ 2221'C, mm21'C, mm21'A, mmm1'C. \end{cases}$
$Fmmm \equiv D_{2h}^{23}$	$mmmI \equiv \{D_{2h}^{25-28}\}$	$\begin{cases} m'm'mI, 222I_c, mm2I_c, mm2I_a, mmmI_c, \\ 2221'I, mm21'I, mmm1'I. \end{cases}$
$Immm \equiv D_{2h}^{25}$	$mmmF \equiv \{D_{2h}^{23,24}\}$	$\begin{cases} m'm'mF, 222F_s, mm2F_s, mmmF_s, \\ 2221'F, mm21'F, mmm1'F. \end{cases}$

In each table the first column contains the reciprocal space group which characterizes both the non-magnetic and the magnetic crystal-classes given in the second and third columns on the same line in the table. Both Hermann–Mauguin and Schœnflies notations are used for convenience. The arithmetic crystal-classes of the non-magnetic groups are labelled using de Wolff's adaptation of the Hermann–Mauguin-type symbols. For convenience, the list of space groups belonging to that class is given in Schœnflies notation in braces. The arithmetic crystal-classes of magnetic space groups are labelled in a de Wolff-type adaptation of the notation of Belov *et al*.

The arithmetic crystal-classes of magnetic space groups are very important for classifying the translational strata of irreducible co-representations. Deriving the auxiliary non-magnetic group of each magnetic space group and its corresponding reciprocal group as described in section 2, we reached the conclusion that a given reciprocal space group characterizes an arithmetic crystal-class of non-magnetic space groups as well as up to 23 (depending on the case) arithmetic crystal-classes of magnetic space groups. We can then categorize magnetic arithmetic crystal-classes according to their reciprocal space group.

4. Adaptation of a theorem of Burnside to co-representations and their enumeration

Once the translational strata of irreducible co-representations have been determined, the inequivalent types of irreducible co-representations contained within each stratum have to be enumerated. This can be done in a way similar to that used for space-group representations,

Table 4. Arithmetic crystal-classes of tetragonal space groups.

Reciprocal space group	Non-magnetic arithmetic crystal-classes	Magnetic arithmetic crystal-classes
$P4 \equiv C_4^1$	$4P \equiv \{C_4^{1-4}\}$	$\bar{4}'P$, $4/m'P$
$I4 \equiv C_4^5$	$4I \equiv \{C_4^{5-6}\}$	$\bar{4}'I$, $4/m'I$
$P\bar{4} \equiv S_4^1$	$\bar{4}P \equiv \{S_4^1\}$	$4'P$, $4'/m'P$
$I\bar{4} \equiv S_4^2$	$\bar{4}I \equiv \{S_4^2\}$	$4'I$, $4'/m'I$
$P4/m \equiv C_{4h}^1$	$4/mP \equiv \{C_{4h}^{1-4}\}$	$4'/mP$, $4P_c$, $\bar{4}P_c$, $4/mP_c$, $4P_C$, $\bar{4}P_C$, $4/mP_C$, $4P_I$, $\bar{4}P_I$, $4/mP_I$, $41'P$, $\bar{4}1'P$, $4/m1'P$.
$I4/m \equiv C_{4h}^5$	$4/mI \equiv \{C_{4h}^{5-6}\}$	$4'/mI$, $4I_c$, $\bar{4}I_c$, $4/mI_c$, $41'I$, $\bar{4}1'I$, $4/m1'I$
$P422 \equiv D_4^1$	$422P \equiv \{D_4^{1-8}\}$	$4m'm'P$, $\bar{4}'2m'P$, $\bar{4}'m'2P$, $4/m'm'm'P$
$I422 \equiv D_4^9$	$422I \equiv \{D_4^{9-10}\}$	$4m'm'I$, $\bar{4}'2m'I$, $\bar{4}'m'2I$, $4/m'm'm'I$
$P4mm \equiv C_{4v}^1$	$4mmP \equiv \{C_{4v}^{1-8}\}$	$42'2'P$, $\bar{4}'2'mP$, $\bar{4}'m2'P$, $4/m'mmP$
$I4mm \equiv C_{4v}^9$	$4mmI \equiv \{C_{4v}^{9-12}\}$	$42'2'I$, $\bar{4}'2'mI$, $\bar{4}'m2'I$, $4/m'mmI$
$P\bar{4}2m \equiv D_{2d}^1$	$\bar{4}2mP \equiv \{D_{2d}^{1-4}\}$	$4'22'P$, $4'm'mP$, $\bar{4}m'2'P$, $4'/m'm'mP$
$P\bar{4}m2 \equiv D_{2d}^5$	$\bar{4}m2P \equiv \{D_{2d}^{5-8}\}$	$4'2'2P$, $4'mm'P$, $\bar{4}2'm'P$, $4'/m'mm'P$
$I\bar{4}m2 \equiv D_{2d}^9$	$\bar{4}2mI \equiv \{D_{2d}^{11,12}\}$	$4'22'I$, $4'm'mI$, $\bar{4}m'2'I$, $4'/m'm'mI$
$I\bar{4}2m \equiv D_{2d}^{11}$	$\bar{4}m2I \equiv \{D_{2d}^{9,10}\}$	$4'2'2I$, $4'mm'I$, $\bar{4}2'm'I$, $4'/m'mm'I$
$P4/mmm \equiv D_{4h}^1$	$4/mmmP \equiv \{D_{4h}^{1-16}\}$	$4'/mm'mP$, $4'/mmm'P$, $4/mm'm'P$, $422P_c$, $4mmP_c$, $\bar{4}2mP_c$, $\bar{4}m2P_c$, $4/mmmP_c$, $422P_C$, $4mmP_C$, $\bar{4}2mP_C$, $\bar{4}m2P_C$, $4/mmmP_C$, $422P_I$, $4mmP_I$, $\bar{4}2mP_I$, $\bar{4}m2P_I$, $4/mmmP_I$, $4221'P$, $4mm1'P$, $\bar{4}2m1'P$, $\bar{4}m21'P$, $4/mmm1'P$.
$I4/mmm \equiv D_{4h}^{17}$	$4/mmmI \equiv \{D_{4h}^{17-20}\}$	$4'/mm'mI$, $4'/mmm'I$, $4/mm'm'I$, $422I_c$, $4mmI_c$, $\bar{4}2mI_c$, $\bar{4}m2I_c$, $4/mmmI_c$, $4221'I$, $4mm1'I$, $\bar{4}2m1'I$, $\bar{4}m21'I$, $4/mmm1'I$.

Table 5. Arithmetic crystal-classes of trigonal space groups.

Reciprocal space group	Non-magnetic arithmetic crystal-classes	Magnetic arithmetic crystal-classes
$P3 \equiv C_3^1$	$3P \equiv \{C_3^{1-3}\}$	$\bar{3}'P$
$R3 \equiv C_3^4$	$3R \equiv \{C_3^4\}$	$\bar{3}'R$
$P\bar{3} \equiv S_6^1$	$\bar{3}P \equiv \{S_6^1\}$	$3P_c$, $\bar{3}P_c$, $31'P$, $\bar{3}1'P$
$R\bar{3} \equiv S_6^2$	$\bar{3}R \equiv \{S_6^2\}$	$3R_I$, $\bar{3}R_I$, $31'R$, $\bar{3}1'R$
$P312 \equiv D_3^1$	$321P \equiv \{D_3^{2,4,6}\}$	$3m'1P$, $\bar{3}'m'1P$
$P321 \equiv D_3^2$	$312P \equiv \{D_3^{1,3,5}\}$	$31m'P$, $\bar{3}'1m'P$
$R32 \equiv D_3^7$	$32R \equiv \{D_3^7\}$	$3m'R$, $\bar{3}'m'R$
$P3m1 \equiv C_{3v}^1$	$31mP \equiv \{C_{3v}^{2,4}\}$	$312'P$, $\bar{3}'1mP$
$P31m \equiv C_{3v}^2$	$3m1P \equiv \{C_{3v}^{1,3}\}$	$32'1P$, $\bar{3}'m1P$
$R3m \equiv C_{3v}^5$	$3mR \equiv \{C_{3v}^{5,6}\}$	$32'R$, $\bar{3}'mR$
$P\bar{3}1m \equiv D_{3d}^1$	$\bar{3}m1P \equiv \{D_{3d}^{3,4}\}$	$\bar{3}m'1P$, $321P_c$, $3m1P_c$, $\bar{3}m1P_c$, $321'P$, $3m1'P$, $\bar{3}m1'P$
$P\bar{3}m1 \equiv D_{3d}^3$	$\bar{3}1mP \equiv \{D_{3d}^{1,2}\}$	$\bar{3}1m'P$, $312P_c$, $31mP_c$, $\bar{3}1mP_c$, $31'2P$, $31'mP$, $\bar{3}1'mP$
$R\bar{3}m \equiv D_{3d}^5$	$\bar{3}mR \equiv \{D_{3d}^5\}$	$\bar{3}m'R$, $32R_I$, $3mR_I$, $\bar{3}mR_I$, $321'R$, $3m1'R$, $\bar{3}m1'R$

i.e. by using an extension of the theorem of Burnside [31] which states that the sum of the

Table 6. Arithmetic crystal-classes of hexagonal space groups.

Reciprocal space group	Non-magnetic arithmetic crystal-classes	Magnetic arithmetic crystal-classes
$P6 \equiv C_6^1$	$6P \equiv \{C_6^{1-6}\}$	$\bar{6}'P$, $6/m'P$
$P\bar{6} \equiv C_{3h}^1$	$\bar{6}P \equiv \{C_{3h}^1\}$	$6'P$, $6'/mP$
$P6/m \equiv C_{6h}^1$	$6/mP \equiv \{C_{6h}^{1,2}\}$	$6'/m'P$, $6P_c$, $\bar{6}P_c$, $6/mP_c$, $61'P$, $\bar{6}1'P$, $6/m1'P$
$P622 \equiv D_6^1$	$622P \equiv \{D_6^{1-6}\}$	$6m'm'P$, $\bar{6}'m'2P$, $\bar{6}'2m'P$
$P6mm \equiv C_{6v}^1$	$6mmP \equiv \{C_{6v}^{1-4}\}$	$62'2'P$, $\bar{6}'m2'P$, $\bar{6}'2'm'P$, $6/m'mmP$
$P\bar{6}m2 \equiv D_{3h}^1$	$\bar{6}2mP \equiv \{D_{3h}^{3,4}\}$	$6'22'P$, $6'm'mP$, $\bar{6}m'2'P$, $6'/mm'mP$
$P\bar{6}2m \equiv D_{3h}^3$	$\bar{6}m2P \equiv \{D_{3h}^{1,2}\}$	$6'2'2P$, $6'mm'P$, $\bar{6}2'm'P$, $6'/mmm'P$
$P6/mmm \equiv D_{6h}^1$	$6/mmm \equiv \{D_{6h}^{1-4}\}$	$6'/m'm'mP$, $6'/m'mm'P$, $6/mm'm'P$, $6/m'm'm'P$, $622P_c$, $6mmP_c$, $\bar{6}m2P_c$, $\bar{6}2mP_c$, $6/mmmP_c$, $6221'P$, $6mm1'P$, $\bar{6}m21'P$, $\bar{6}2m1'P$, $6/mmm1'P$.

Table 7. Arithmetic crystal-classes of cubic space groups.

Reciprocal space group	Non-magnetic arithmetic crystal-classes	Magnetic arithmetic crystal-classes
$P23 \equiv T^1$	$23P \equiv \{T^{1,4}\}$	$m'3P$
$F23 \equiv T^2$	$23I \equiv \{T^{3,5}\}$	$m'3I$
$I23 \equiv T^3$	$23F \equiv \{T^2\}$	$m'3F$
$Pm\bar{3} \equiv T_h^1$	$m\bar{3}P \equiv \{T_h^{1,2,6}\}$	$23P_I$, $m3P_I$, $23'P$, $m3'P$
$Fm\bar{3} \equiv T_h^3$	$m\bar{3}I \equiv \{T_h^{5,7}\}$	$23'I$, $m3'I$
$Im\bar{3} \equiv T_h^5$	$m\bar{3}F \equiv \{T_h^{3,4}\}$	$23F_s$, $m3F_s$, $23'F$, $m3'F$
$P432 \equiv O^1$	$432P \equiv \{O^{1,2,6,7}\}$	$\bar{4}'3m'P$, $m'3m'P$
$F432 \equiv O^3$	$432I \equiv \{O^{5,8}\}$	$\bar{4}'3m'I$, $m'3m'I$
$I432 \equiv O^5$	$432F \equiv \{O^{3,4}\}$	$\bar{4}'3m'F$, $m'3m'F$
$P\bar{4}3m \equiv T_d^1$	$\bar{4}3mP \equiv \{T_d^{1,4}\}$	$4'32'P$, $m'3mP$
$F\bar{4}3m \equiv T_d^2$	$\bar{4}3mI \equiv \{T_d^{3,6}\}$	$4'32'I$, $m'3mI$
$I\bar{4}3m \equiv T_d^3$	$\bar{4}3mF \equiv \{T_d^{2,5}\}$	$4'32'F$, $m'3mF$
$Pm\bar{3}m \equiv O_h^1$	$m\bar{3}mP \equiv \{O_h^{1-4}\}$	$m3m'P$, $432P_I$, $\bar{4}3mP_I$, $m3mP_I$, $43'2P$, $\bar{4}3'mP$, $m3'mP$
$Fm\bar{3}m \equiv O_h^5$	$m\bar{3}mI \equiv \{O_h^{9,10}\}$	$m3m'I$, $43'2I$, $\bar{4}3'mI$, $m3'mI$
$Im\bar{3}m \equiv O_h^9$	$m\bar{3}mF \equiv \{O_h^{5-8}\}$	$m3m'F$, $432F_s$, $\bar{4}3mF_s$, $m3mF_s$, $43'2F$, $\bar{4}3'mF$, $m3'mF$

squares of the dimensions of the irreducible representations of a group is equal to the order of the group. However, space groups are infinite groups and hence direct application of Burnside's theorem is inappropriate.

Furthermore, in its original form Burnside's theorem cannot be applied directly to magnetic groups as it is not valid for co-representations. To adapt this theorem to co-representations the possible types of relationship between the co-representations of the magnetic group and the irreducible representations of the non-magnetic halving subgroup are relevant. These can be summarized by the following correlation table in which D are co-representations of the magnetic group, M, while $\Delta(u)$ and $\bar{\Delta}(u) = \Delta(a_0^{-1}ua_0)^* \not\equiv \Delta(u)$ are ordinary representations of the subgroup, H:

M	H
${}^aD_\alpha$	Δ_α
${}^bD_\beta$	$2\Delta_\beta$
${}^cD_\gamma$	$\Delta_\gamma \oplus \bar{\Delta}_\gamma$

These three splitting patterns respectively correspond to Wigner's types a, b and c [3]. The big difference between the correlation of co-representations with ordinary representations of the halving subgroup and correlations between ordinary representations of ordinary, non-magnetic, groups lies in the restriction that a given representation Δ_i of H can *only* derive by subduction from a *single* co-representation D_i of M and not from one or two such co-representations as the Frobenius reciprocity theorem would suggest for ordinary representations.

Writing Burnside's theorem in the form

$$\sum_{i=1}^{s} |\Delta_i|^2 = |H| \tag{7}$$

where $|\Delta_i|$ is the dimension of Δ_i, the complete set of s irreducible representations of H can be partitioned into three according to whether the irreducible representation is obtained by subduction from a type a, type b or type c co-representation of M. Given that the three splitting patterns, respectively, imply the relationships $|{}^aD_\alpha| = |\Delta_\alpha|$, $|{}^bD_\beta| = 2|\Delta_\beta|$ and $|{}^cD_\gamma| = 2|\Delta_\gamma| = 2|\bar{\Delta}_\gamma|$ and that $\Delta_\gamma \not\equiv \bar{\Delta}_\gamma$, $|\Delta_i|^2$ can be replaced in equation (7) by the following combination of $|D_i|^2$ terms which has coefficients which vary with the Wigner type:

$$\sum_{\alpha=1}^{l} |{}^aD_\alpha|^2 + \tfrac{1}{4}\sum_{\beta=1}^{m} |{}^bD_\beta|^2 + \tfrac{1}{2}\sum_{\gamma=1}^{n} |{}^cD_\gamma|^2 = |H| = \tfrac{1}{2}|M| \tag{8}$$

where $l + m + 2n$ is equal to the total number s of irreducible representations of H. This modified form of Burnside's theorem was tested on all 90 magnetic point groups and their irreducible co-representations were found to satisfy it without exception.

The co-representations of magnetic space groups will also obey this rule but it is of little practical value in its present form because the number s of irreducible co-representations is infinite. However, Boyle found in a study of the completeness problem in the definition of projective representations that Burnside's formula applied to each class of projective representations separately and hence the formula applied to the double-valued representations of a double group separately from the single-valued representations and also, because space-group representations could be constructed from projective representations of point groups, the enumeration of the complete set of representations of a given space group should be amenable to this type of analysis.

In practice, a Burnside-type formula was obtained for ordinary space groups by recognizing that although the total number of irreducible representations was infinite, the number corresponding to a given set of the arbitrary parameters (i.e. the number of a particular translational type) was finite and that their dimensions obeyed the formula

$$\sum_{i=1}^{s} |\Delta_i(\mathcal{T})|^2 = |P_H|^2/|S_\mathcal{T}| = |P_H| \times |P_R|/|S_\mathcal{T}| \tag{9}$$

where $|P_H|$ is the order of the point group of the space group, H, $|P_R|$ is the order of the point group of the reciprocal space group, R, and $|S_\mathcal{T}|$ is the order of the stabilizer (or site-symmetry group), $S_\mathcal{T}$, of a point in the Wyckoff set characterizing the translational stratum $\mathcal{T}$ to which the particular set of values of the parameters $\{p, q, r\}$ belongs. Equation (9) was obtained by induction and tested for all ordinary space groups. It can be recognized as a generalization of the original Burnside equation (7) by considering the set of representations with the full translational symmetry of the lattice. These can always be mapped onto the point-group representations and, since for these $S_{\mathcal{T}} = P_H$, equation (9) maps onto equation (7).

The Burnside-like formula for co-representations then follows by replacing the expression for the sum over the squares of the dimensions of the representations by the appropriate Wigner-type-dependent combination of sums of the squares of the co-representations as was used for the magnetic point groups in equation (8):

$$\sum_{\alpha=1}^{l} |{}^{a}D_{\alpha}(\mathcal{T})|^2 + \tfrac{1}{4}\sum_{\beta=1}^{m} |{}^{b}D_{\beta}(\mathcal{T})|^2 + \tfrac{1}{2}\sum_{\gamma=1}^{n} |{}^{c}D_{\gamma}(\mathcal{T})|^2 = |P_H| \times |P_R|/|S_{\mathcal{T}}|. \tag{10}$$

The choice of the right-hand side to be the second of those given in equation (9) is heuristic. Note that in magnetic space groups $|P_R|$ is not necessarily equal to $|P_H|$ as in the case of ordinary space groups and hence equation (10) cannot be simplified to $|P_H|^2/|S_{\mathcal{T}}|$ as in the case of equation (9).

It turns out that this adaptation of Burnside's theorem is more than just a way of checking that no co-representation has been omitted or counted twice from each stratum because there is only a limited number of ways of satisfying the Diophantine equation (10) and there is therefore only a limited number of patterns of co-representations which can occur. Given that b- and c-type co-representations must be of even dimension, the weighted sums of squares of the dimensions of the a- and b-type co-representations must each be a sum of squares of natural numbers while the corresponding sum for the c-type co-representations must be twice such a sum of squares of natural numbers. In practice, no example exists of two different Wigner types of co-representation existing in the same stratum for all of the triclinic, monoclinic and orthorhombic groups and no example of a stratum containing all three different Wigner types has been found. The Diophantine solutions to equation (10) have been found for the cases when the right-hand side is 1, 2, 3 or 4 and will be published elsewhere [32].

5. Illustrative examples

Two examples of character tables of full-group co-representations of black-and-white space groups are given which illustrate how the above theory may be applied. For simplicity the examples are restricted to single-valued co-representations but there is in principle no difficulty in extending the results to double-valued co-representations.

5.1. Example 1. $C_{2h}^3(C_{2h}^1) \equiv P_C 2/m \equiv \mathrm{III}_{10}^{49}$

This is a black-and-white group of considerable practical importance as the symmetry group of the α-phase of solid oxygen, α-O_2. This phase is stable from 0 K to 23.876 K at which temperature a second-order transition to the β-phase takes place. This transition is due to the anti-ferromagnetic ordering being destroyed by the thermal motion. This is, however, restricted to motion of the molecules about an axis or in a plane until 43.818 K when a first-order transition to the γ-phase takes place. At 54.39 K the solid melts.

The first symbol for the magnetic group is a Schœnflies-type notation of the form $G(H)$ showing that the non-magnetic subgroup is $H = C_{2h}^1 \equiv P2/m$ and that the isomorphic non-magnetic group is $G = C_{2h}^3 \equiv C2/m$. Since the point groups of G and H are the same, H is a *klassengleiche* subgroup of G and hence the magnetic group M is of *klassengleiche* type.

The second symbol is an adaptation to magnetic groups of the international notation [29, 30] in which the lattice symbol P_C denotes a black-and-white lattice while the point-group part, $2/m$, being unprimed, indicates that the occurrence of the time inversion is connected with the translations rather than with the particular point-group elements. In the third symbol the Cyrillic letter III invokes the alternative name 'Shubnikov groups' for magnetic groups [33] and the numerical subscript and superscript are defined in the original enumeration [29, 30].

The group G is the holosymmetric, symmorphic, side-centred monoclinic space group, C_{2h}^3, while the subgroup H is the holosymmetric, symmorphic, primitive monoclinic space group, C_{2h}^1. The relationship between these two groups is often regarded as a 'decentring'. The auxiliary group is then given by equation (6) as isomorphic to H and hence the reciprocal space group is also C_{2h}^1 (line 5 of table 2).

The first Brillouin zone is chosen as a primitive monoclinic unit cell and is the same for the magnetic group $C_{2h}^3(C_{2h}^1)$ and the auxiliary non-magnetic group C_{2h}^1 since both groups have a common reciprocal space group C_{2h}^1.

The characters of the co-representations of $C_{2h}^3(C_{2h}^1)$ are given in table 8. The method adopted for storing the information is similar to that used for ordinary space groups [34, 35]. The elements of the group are presented in the form of a coset decomposition with respect to the translational subgroup. Only one representative of each coset is given and Seitz notation [36] is used. For convenience the point-group parts of the elements are noted above each entry and the anti-unitary cosets can be identified by the presence of the time inversion θ. The dimensions of the co-representations are given by the numerical factors in the column corresponding to the coset of pure translations, i.e. the first column of the main part of the table.

The full-group characters are given in terms of functions (denoted by I) of primitive translations v_x, v_y and v_z which are invariant under the action of point-group operations and can be written as follows:

$$\begin{aligned}
&I_Z = (-1)^{v_y} \qquad I_B = (-1)^{v_z} \qquad I_Y = (-1)^{v_x} \\
&I_C = (-1)^{v_x+v_y} \qquad I_D = (-1)^{v_y+v_z} \\
&I_A = (-1)^{v_z+v_x} \qquad I_E = (-1)^{v_x+v_y+v_z} \\
&I_\Lambda = \cos 2\pi p v_y \qquad I_W = (-1)^{v_x} \cos 2\pi p v_y \\
&I_V = (-1)^{v_z} \cos 2\pi p v_y \qquad I_U = (-1)^{v_z+v_x} \cos 2\pi p v_y \\
&I_F = \cos\{2\pi(p v_z + q v_x)\} \qquad I_G = (-1)^{v_y} \cos\{2\pi(p v_z + q v_x)\} \\
&I_O = \tfrac{1}{2}[\cos\{2\pi(p v_x + q v_y + r v_z)\} + \cos\{2\pi(p v_x - q v_y + r v_z)\}].
\end{aligned} \tag{11}$$

This set of invariant character functions is common to all magnetic space groups of the arithmetic class $2/mP_C$, i.e. the groups $P_C 2/m$, $P_C 2_1/m$, $P2/c$ and $P_C 2_1/c$, and to the other 12 magnetic arithmetic crystal-classes of space groups which have $C_{2h}^1 \equiv P2/m$ as reciprocal space group (cf table 2).

The character functions which are not invariant to the point-group elements are denoted by other letters of the alphabet including accents and primes to give sufficient variety:

$$\begin{aligned}
&g_y = \cos\{2\pi p(v_y + \tfrac{1}{2})\} \qquad \ddot{u}_y = (-1)^{v_z} \cos\{2\pi p(v_y + \tfrac{1}{2})\} \\
&\ddot{U}_y'' = \cos[2\pi\{p v_z + q(v_x + \tfrac{1}{2})\}] \\
&J_y = \tfrac{1}{2}[\cos[2\pi\{p(v_x + \tfrac{1}{2}) + q(v_y + \tfrac{1}{2}) + r v_z] + \cos[2\pi\{p(v_x + \tfrac{1}{2}) - q(v_y + \tfrac{1}{2}) + r v_z\}]].
\end{aligned} \tag{12}$$

The strata of irreducible co-representations are listed in the left-hand column of the main part of the character table and individual irreducible co-representations are obtained by choosing specific values for such variable parameters $\{p, q, r\}$ as may occur. Inequivalent co-representations within a stratum are labelled with the same capital letter and the sequence

Table 8. Character table of $C_{2h}^3(C_{2h}^1) \equiv P_C 2/m \equiv \mathrm{III}_{10}^{49}$.

$C_{2h}^3(C_{2h}^1)$	E	C_2	S_2	σ_h	θ	θC_2	θS_2	$\theta\sigma_h$
$P_C 12/m1$	$\overbrace{\{xyz\|000\}}$	$\overbrace{\{\bar{x}y\bar{z}\|000\}}$	$\overbrace{\{\bar{x}\bar{y}\bar{z}\|000\}}$	$\overbrace{\{x\bar{y}z\|000\}}$	$\overbrace{\theta\{xyz\|\frac{1}{2}\frac{1}{2}0\}}$	$\overbrace{\theta\{\bar{x}y\bar{z}\|\frac{1}{2}\frac{1}{2}0\}}$	$\overbrace{\theta\{\bar{x}\bar{y}\bar{z}\|\frac{1}{2}\frac{1}{2}0\}}$	$\overbrace{\theta\{x\bar{y}z\|\frac{1}{2}\frac{1}{2}0\}}$
$^a\Gamma_1^+$	1	1	1	1	1	1	1	1
$^a\Gamma_2^+$	1	-1	1	-1	1	-1	1	-1
$^a\Gamma_1^-$	1	1	-1	-1	1	1	-1	-1
$^a\Gamma_2^-$	1	-1	-1	1	1	-1	-1	1
$^cZ_1$	$2I_Z$	$2I_Z$	0	0	0	0	0	0
$^cZ_2$	$2I_Z$	$-2I_Z$	0	0	0	0	0	0
$^aB_1^+$	I_B	I_B	I_B	I_B	I_B	I_B	I_B	I_B
$^aB_2^+$	I_B	$-I_B$	I_B	$-I_B$	I_B	$-I_B$	I_B	$-I_B$
$^aB_1^-$	I_B	I_B	$-I_B$	$-I_B$	I_B	I_B	$-I_B$	$-I_B$
$^aB_2^-$	I_B	$-I_B$	$-I_B$	I_B	I_B	$-I_B$	$-I_B$	I_B
$^cY_1$	$2I_Y$	0	0	$2I_Y$	0	0	0	0
$^cY_2$	$2I_Y$	0	0	$-2I_Y$	0	0	0	0
$^cC_1^+$	$2I_C$	0	$2I_C$	0	0	0	0	0
$^cC_1^-$	$2I_C$	0	$-2I_C$	0	0	0	0	0
$^cD_1$	$2I_D$	$2I_D$	0	0	0	0	0	0
$^cD_2$	$2I_D$	$-2I_D$	0	0	0	0	0	0
$^cA_1$	$2I_A$	0	0	$2I_A$	0	0	0	0
$^cA_2$	$2I_A$	0	0	$-2I_A$	0	0	0	0
$^cE_1^+$	$2I_E$	0	$2I_E$	0	0	0	0	0
$^cE_1^-$	$2I_E$	0	$-2I_E$	0	0	0	0	0
$^a\Lambda_1(p)$	$2I_\Lambda$	$2I_\Lambda$	0	0	$2g_y$	$2g_y$	0	0
$^a\Lambda_2(p)$	$2I_\Lambda$	$-2I_\Lambda$	0	0	$2g_y$	$-2g_y$	0	0
$^cW_1(p)$	$4I_W$	0	0	0	0	0	0	0
$^aV_1(p)$	$2I_V$	$2I_V$	0	0	$2\ddot{u}_y$	$2\ddot{u}_y$	0	0
$^aV_2(p)$	$2I_V$	$-2I_V$	0	0	$2\ddot{u}_y$	$-2\ddot{u}_y$	0	0
$^cU_1(p)$	$4I_U$	0	0	0	0	0	0	0
$^aF_1(p,q)$	$2I_F$	0	0	$2I_F$	$2\ddot{U}_y''$	0	0	$2\ddot{U}_y''$
$^aF_2(p,q)$	$2I_F$	0	0	$-2I_F$	$2\ddot{U}_y''$	0	0	$-2\ddot{U}_y''$
$^cG_1(p,q)$	$4I_G$	0	0	0	0	0	0	0
$^aO_1(p,q,r)$	$4I_O$	0	0	0	$4J_y$	0	0	0

of co-representations is specially chosen to be that of the Wyckoff sets of points in the reciprocal space group. This also facilitates the identification of the stabilizers of each stratum since the site symmetry groups of Wyckoff sets are available in all editions of *International Tables* [20, 23, 24]. The orbits are labelled in accordance with the standard notation [11, 12, 14, 17]. The pre-superscripts a, b and c denote the Wigner type of the co-representations while the numerical subscripts label the inequivalent co-representations within a given translational stratum. The post-superscripts '$+$' and '$-$' are used in centrosymmetric groups to distinguish between the even and odd symmetry of the co-representations under space inversion.

The trivariant translational stratum in table 8, $O(p, q, r)$, corresponds to the Wyckoff set, labelled o, which is the set of points with trivial site-symmetry in direct space. This describes a set of general points in the first Brillouin zone and classifies an orbit of general co-representations [37]. The divariant translational strata, labelled $F(p, q)$ and $G(p, q)$, are classified by the Wyckoff sets of points m and n, respectively, which describe two families of planes. The univariant strata, $\Lambda(p)$, $W(p)$, $V(p)$ and $U(p)$, are, respectively, classified by Wyckoff sets i, j, k and l which correspond to lines in the Brillouin zone. Since these lines are not located at the intersections of symmetry planes they are referred to as isolated lines of symmetry which in this case are twofold axes of symmetry. The remaining strata, Γ, Z, B, Y, C, D, A and E, have no degrees of freedom and are classified by special points in the Brillouin zone corresponding to Wyckoff points a to h, respectively.

Comparison with the little-group character tables of Miller and Love [12] shows good agreement for the invariant and univariant strata of irreducible co-representations except where they omitted the little-group analogues of the divariant strata $F_1(p, q)$, $F_2(p, q)$ and $G_1(p, q)$ and the trivariant stratum ${}^aO_1(p, q, r)$.

5.2. Example 2. $C_4^1(C_2^1) \equiv P4' \equiv \mathrm{III}_{75}^3$

This is a group of *zellengleiche* type in which the groups G and H are both space groups only having pure rotations, translations and their combinations. Neither group is centrosymmetric and, according to equation (5), the auxiliary group A is $S_4^1 \equiv P\bar{4}$. It is a self-reciprocal group (line 3 of table 4) and also lacks a centre of symmetry. Hence the Brillouin zone for both groups S_4^1 and $C_4^1(C_2^1)$ has no centre of symmetry and can be chosen as a primitive tetragonal unit cell. Its special symmetries are characterized by the eight Wyckoff strata of sets of points of the reciprocal group S_4^1. The character table is given in table 9.

A general set, labelled h, classifies the stratum of the general co-representations $O(p, q, r)$ which are also of Wigner type c. The Wyckoff sets e, f and g classify lines in the Brillouin zone. The corresponding univariant translational strata $\Lambda(p)$, $V(p)$ and $W(p)$ contain co-representations of Wigner type c. The sets a, b, c and d classify points in the Brillouin zone and correspond to the invariant strata Γ, Z, M and A.

Miller and Love [12] give four additional little-group co-representations of Wigner type c labelled by the points X and R with coordinates $(0\frac{1}{2}0)$ and $(0\frac{1}{2}\frac{1}{2})$, respectively. However, X and R belong to the line labelling the stratum $W(p)$ and are not special points in the appropriate Brillouin zone since they are not located at the intersections of lines of symmetry with another line or plane of symmetry. The co-representations in question are generated by putting $p = 0$ and $p = \frac{1}{2}$ in ${}^cW_1(p)$ and ${}^cW_2(p)$. Hence inclusion of X and R produces extraneous entries because the Brillouin zone used in [12] belongs to the holosymmetric group C_{4h}^1 which has additional Wyckoff orbits e and f corresponding to the points X and R. This also causes extraneous entries to occur in the little-group character table of the irreducible representations of S_4^1.

Table 9. Character table of $C_4^1(C_2^1) \equiv P4' \equiv \mathrm{III}_{75}^3$.

$C_4^1(C_2^1)$	E	C_2	θC_4	θC_4^3
$P4'$	$\{xyz\|000\}$	$\{\bar{x}\bar{y}z\|000\}$	$\theta\{\bar{y}xz\|000\}$	$\theta\{y\bar{x}z\|000\}$
${}^a\Gamma_1$	1	1	1	1
${}^b\Gamma_2$	2	-2	0	0
${}^aZ_1$	I_Z	I_Z	I_Z	I_Z
${}^bZ_2$	$2I_Z$	$-2I_Z$	0	0
${}^aM_1$	I_M	I_M	I_M	I_M
${}^bM_2$	$2I_M$	$-2I_M$	0	0
${}^aA_1$	I_A	I_A	I_A	I_A
${}^bA_2$	$2I_A$	$-2I_A$	0	0
${}^c\Lambda_1(p)$	$2I_\Lambda$	$2I_\Lambda$	0	0
${}^c\Lambda_2(p)$	$2I_\Lambda$	$-2I_\Lambda$	0	0
${}^cV_1(p)$	$2I_V$	$2I_V$	0	0
${}^cV_2(p)$	$2I_V$	$-2I_V$	0	0
${}^cW_1(p)$	$2I_W$	$2I_W$	0	0
${}^cW_2(p)$	$2I_W$	$-2I_W$	0	0
${}^cO_1(p,q,r)$	$4I_O$	0	0	0

The invariant functions occurring in table 9 are

$$\begin{aligned} &I_Z = (-1)^{v_z} \qquad I_M = (-1)^{v_x+v_y} \qquad I_A = (-1)^{v_x+v_y+v_z} \\ &I_\Lambda = \cos 2\pi p v_z \qquad I_V = (-1)^{v_x+v_y} \cos 2\pi p v_z \\ &I_W = \tfrac{1}{2}\{(-1)^{v_y} \mathrm{e}^{2\pi \mathrm{i} p v_z} + (-1)^{v_x} \mathrm{e}^{-2\pi \mathrm{i} p v_z}\} \\ &I_O = \tfrac{1}{2}[\cos\{2\pi(p v_x + q v_y)\}\mathrm{e}^{2\pi \mathrm{i} r v_z} + \cos\{2\pi(p v_y - q v_x)\}\mathrm{e}^{-2\pi \mathrm{i} r v_z}] \end{aligned} \tag{13}$$

and are the same for all non-magnetic and magnetic space groups belonging to the arithmetic crystal classes $\bar{4}P$, $4'P$ and $4'/m'P$ characterized by the reciprocal space group S_4^1.

Another noteworthy feature is the presence of two different Wigner types of co-representation in the same stratum. This never occurs in triclinic, monoclinic or orthorhombic magnetic space groups. The number of inequivalent types of irreducible co-representations contained within each translational stratum is checked using the Burnside-type analysis and the results are given in table 10. Tables such as this are also useful in recognizing which strata of co-representations are related by outer automorphisms of the magnetic group [38]. Two strata can only be regarded as possibly affinely equivalent if the entries for these tables are identical.

6. Conclusions

The concept of the reciprocal space group is particularly useful because it sets the classification problems of irreducible space-group representations and co-representations on a common basis. It explains the special symmetries in the Brillouin zones of both non-magnetic and magnetic crystals and provides a systematic method for classifying, enumerating and labelling both space-group representations, magnetic-group co-representations and the corresponding wavefunctions and energies. It contributes significantly to the classification of space groups themselves as it characterizes an arithmetic crystal-class of non-magnetic space groups and a number of arithmetic crystal-classes of magnetic space groups.

The extension of the Burnside rule to co-representations adds a very convenient check

Table 10. Burnside-type analysis for $C_4^1(C_2^1) \equiv P4' \equiv \mathrm{III}_{75}^3$.

Stratum	$\sum_i \lvert{}^a D_i\rvert^2$	$\frac{1}{4}\sum_i \lvert{}^b D_i\rvert^2$	$\frac{1}{2}\sum_i \lvert{}^c D_i\rvert^2$	Sum	Wyckoff label	Stabilizer $S_{\mathcal{T}}$	$\lvert S_{\mathcal{T}}\rvert$	$\frac{\lvert P_H\rvert \lvert P_R\rvert}{\lvert S_{\mathcal{T}}\rvert}$
Γ	1	1	0	2	a	$\bar{4} \equiv S_4$	4	2
Z	1	1	0	2	b	$\bar{4} \equiv S_4$	4	2
M	1	1	0	2	c	$\bar{4} \equiv S_4$	4	2
A	1	1	0	2	d	$\bar{4} \equiv S_4$	4	2
$\Lambda(p)$	0	0	4	4	e	$2 \equiv C_2$	2	4
$V(p)$	0	0	4	4	f	$2 \equiv C_2$	2	4
$W(p)$	0	0	4	4	g	$2 \equiv C_2$	2	4
$O(p, q, r)$	0	0	8	8	h	$1 \equiv C_1$	1	8

on the completeness of any enumeration of the co-representations belonging to each translational type and shows how the Burnside rule can be applied to a class of finitely-generated groups of infinite order.

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